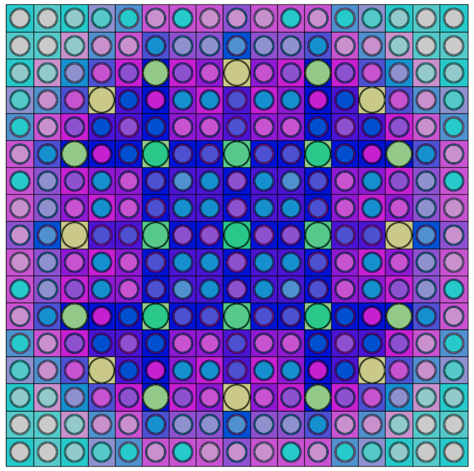
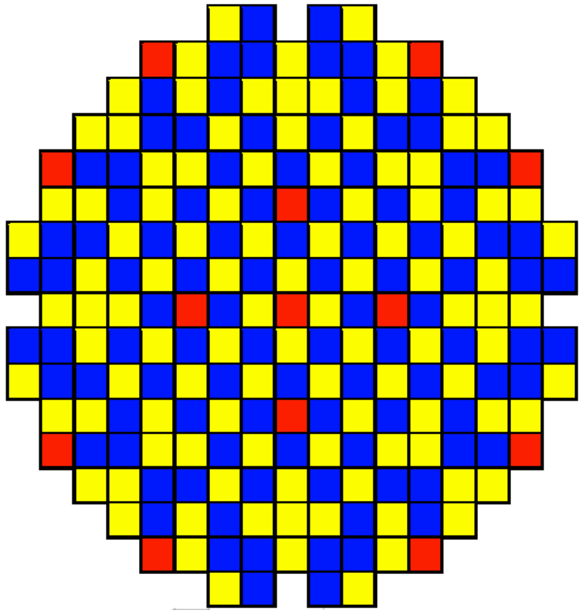


Reactor Simulations With DRAGON For Antineutrino Experiments and Nonproliferation



Christopher Jones

March 18, 2011

As reactors increase in power, new reactor-based particle physics experiments are on the horizon.

-Coherent neutrino scattering
-Weak mixing angle studies
-Neutrino magnetic moment
-Oscillation physics

For all of these, a fast, open sourced, well benchmarked reactor simulation is very valuable!

This is what DRAGON is all about!

Talk Outline

- Example Motivation: Oscillation Experiments
- Overview of Double Chooz Detector
- Overview of Reactors and the DRAGON Code
- The SONGS Antineutrino Rate With DRAGON
- The Takahama-3 Benchmark With DRAGON
- Additional Motivation: Nonproliferation With Antineutrinos

Talk Outline

- Example Motivation: Oscillation Experiments

2 x 2 Neutrino Oscillations

We've learned that neutrinos have mass.

Weak eigenstates are mixtures of the mass eigenstates

$$\begin{pmatrix} \nu_e \\ \nu_\mu \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix}$$

Assume: $\delta m^2 \equiv m_2^2 - m_1^2 \neq 0$

Then, within a pure ν_μ beam at t = 0,

a ν_e component may appear over time!

$$\boxed{P_{app} = \sin^2 2\theta \sin^2 \left(1.27 \frac{\delta m^2 L}{E_\nu}\right)}$$

2 x 2 Neutrino Oscillation Formula

$$P_{app} = \sin^2 2\theta \sin^2 \left(1.27 \frac{\delta m^2 L}{E_\nu}\right)$$

This formula has 2 fundamental parameters:
The mixing angle, θ
the squared mass difference, δm^2

It has 2 experimental parameters:
L, the distance from source to detector
E, the neutrino energy

Experimenter's Choices

Choice #1: Choose L / E such that:

$$\delta m^2 \frac{L}{E_\nu} \approx 1$$

Choice #2: Appearance vs. Disappearance

$$P_{dis} = 1 - \sin^2 2\theta \sin^2 \left(1.27 \frac{\delta m^2 L}{E_\nu} \right)$$

...but we actually have oscillations among three neutrino flavors.

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = \begin{pmatrix} U_{e1} & U_{e2} & U_{e3} \\ U_{\mu 1} & U_{\mu 2} & U_{\mu 3} \\ U_{\tau 1} & U_{\tau 2} & U_{\tau 3} \end{pmatrix} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

Experiment must constrain:

two δm^2 parameters

three Euler angles: $\theta_{12}, \theta_{23}, \theta_{13}$

and potentially one CP-violating term

What we know from experiment...

Flavor eigenstates

PMNS matrix

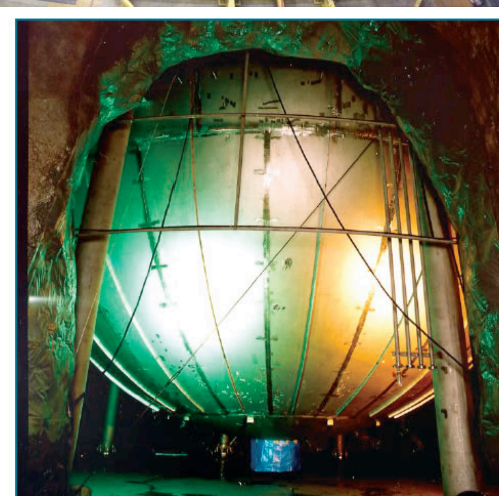
$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} \approx \begin{pmatrix} 0.8 & 0.6 & e^{i\delta}\sin\theta_{13} \\ -0.4 & 0.6 & 0.7 \\ 0.4 & -0.6 & 0.7 \end{pmatrix} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

Mass eigenstates

δm^2_{23} obtained from Super K, K2K, & MINOS

$$\delta m^2_{23} = (2.4 \pm 0.12) \times 10^{-3}\mathrm{eV}^2$$

δm^2_{12} obtained from KamLAND



$$\delta m^2_{12} = (7.65 \pm 0.23) \times 10^{-5}\mathrm{eV}^2$$

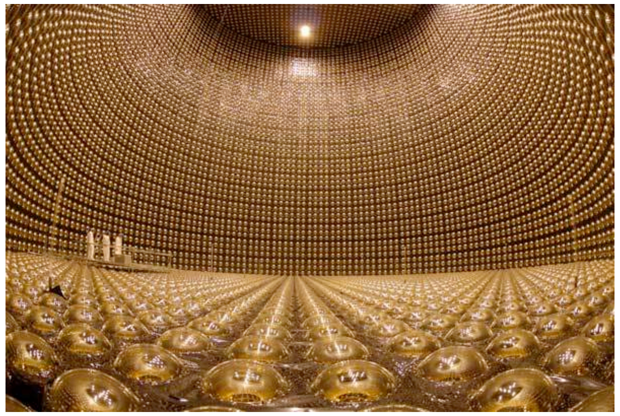
$$\delta m^2_{13} = \delta m^2_{23} + \delta m^2_{12}$$

What we know from experiment...

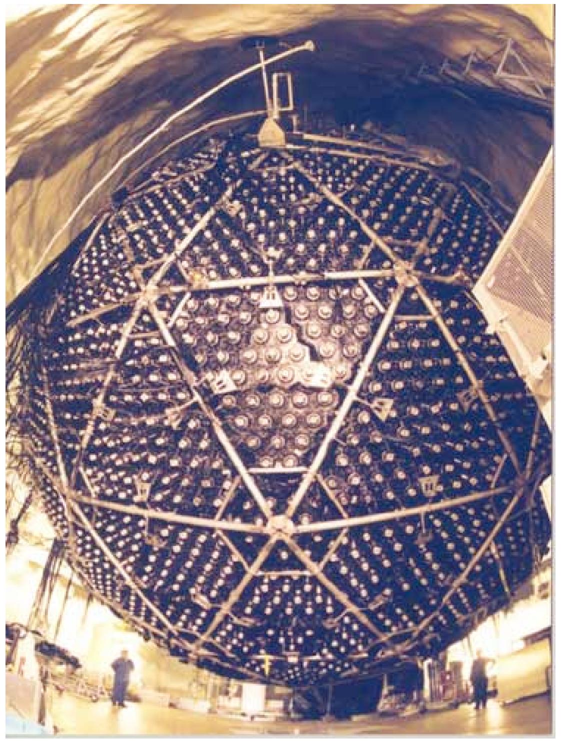
Flavor eigenstates PMNS matrix Mass eigenstates

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} \approx \begin{pmatrix} 0.8 & 0.6 & e^{i\delta}\sin\theta_{13} \\ -0.4 & 0.6 & 0.7 \\ 0.4 & -0.6 & 0.7 \end{pmatrix} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

θ_{23} obtained from Super K, K2K, & MINOS



θ_{12} obtained from solar neutrino experiments, primarily from SNO & Super K



What we know from experiment...

Flavor eigenstates PMNS matrix Mass eigenstates

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} \approx \begin{pmatrix} 0.8 & 0.6 & e^{i\delta}\sin\theta_{13} \\ -0.4 & 0.6 & 0.7 \\ 0.4 & -0.6 & 0.7 \end{pmatrix} \cdot \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

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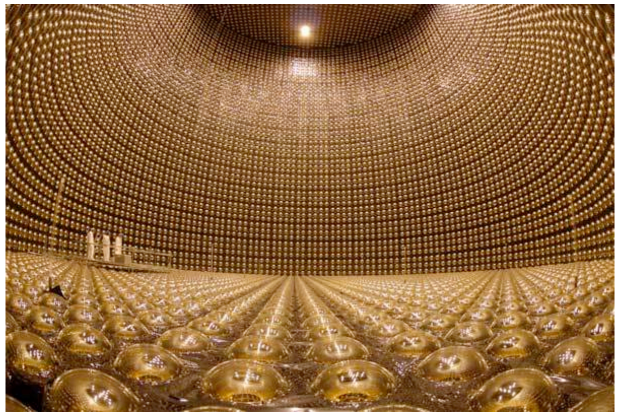

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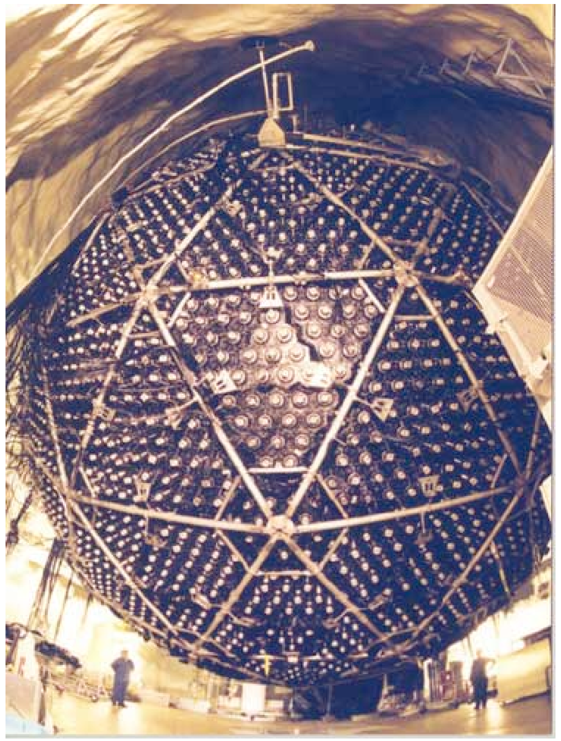


Big problem:

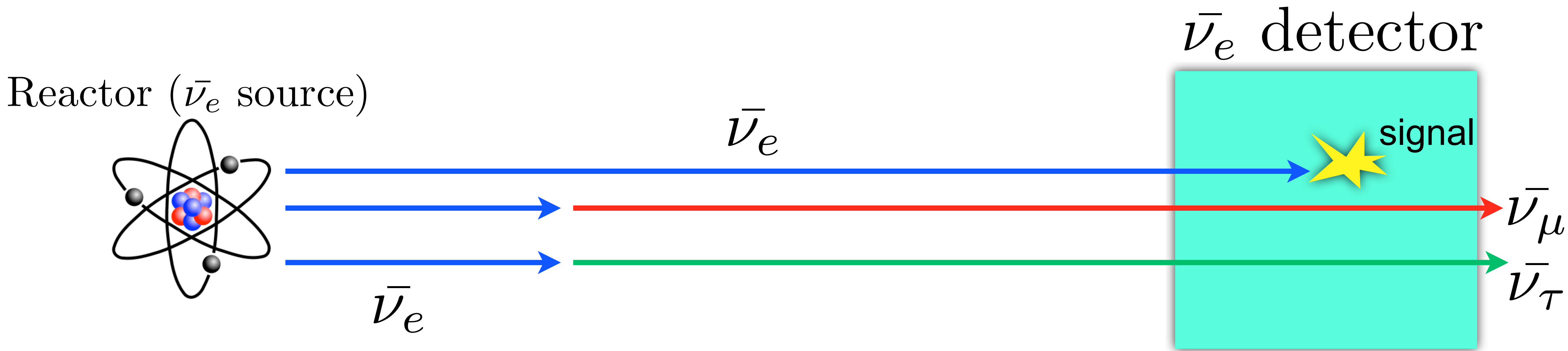
We only have an upper limit for θ_{13}!

$$\sin^2 2\theta_{13} < 0.17$$

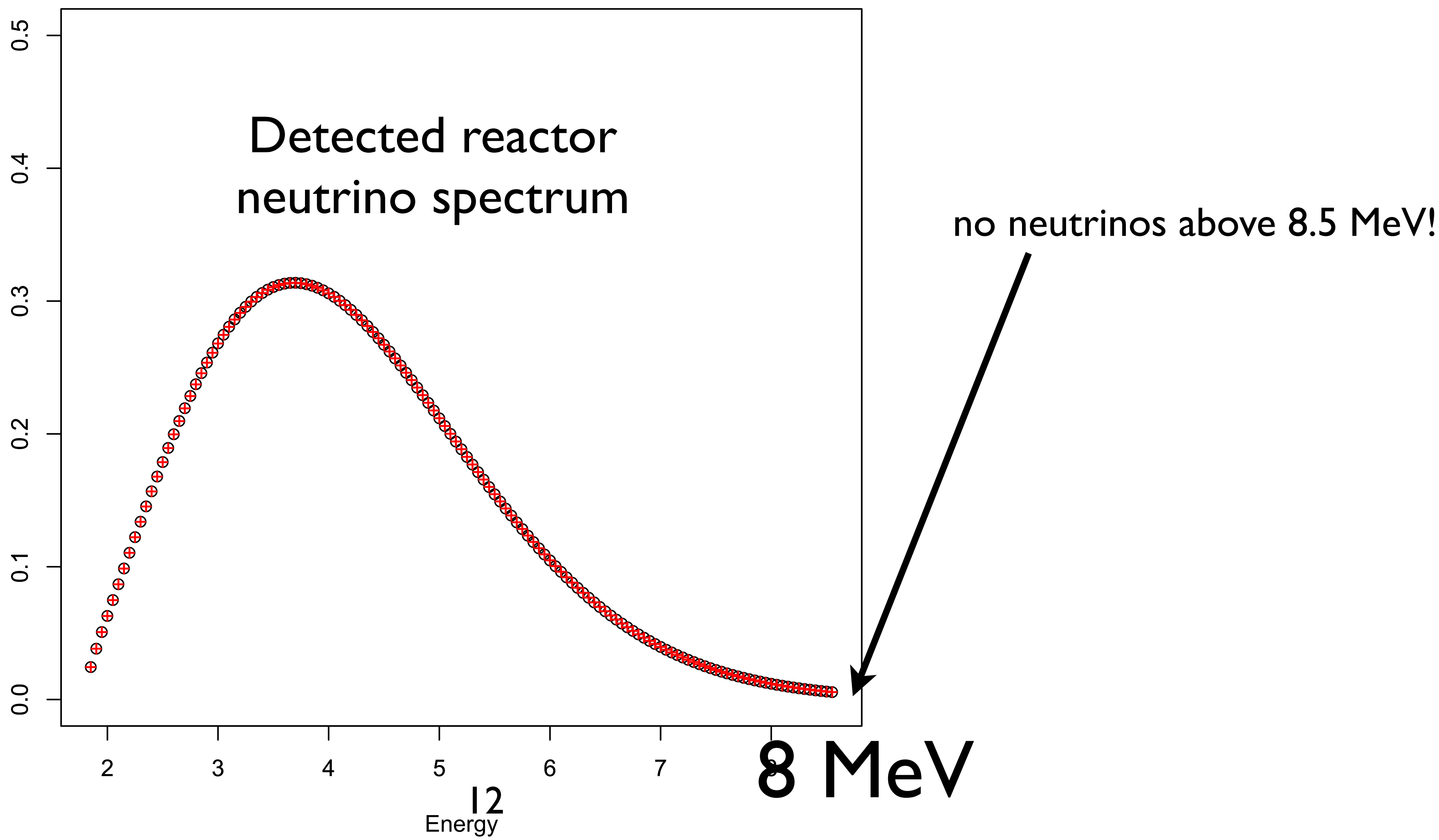
This limit comes CHOOZ, a reactor disappearance experiment.

arXiv:0301017v1

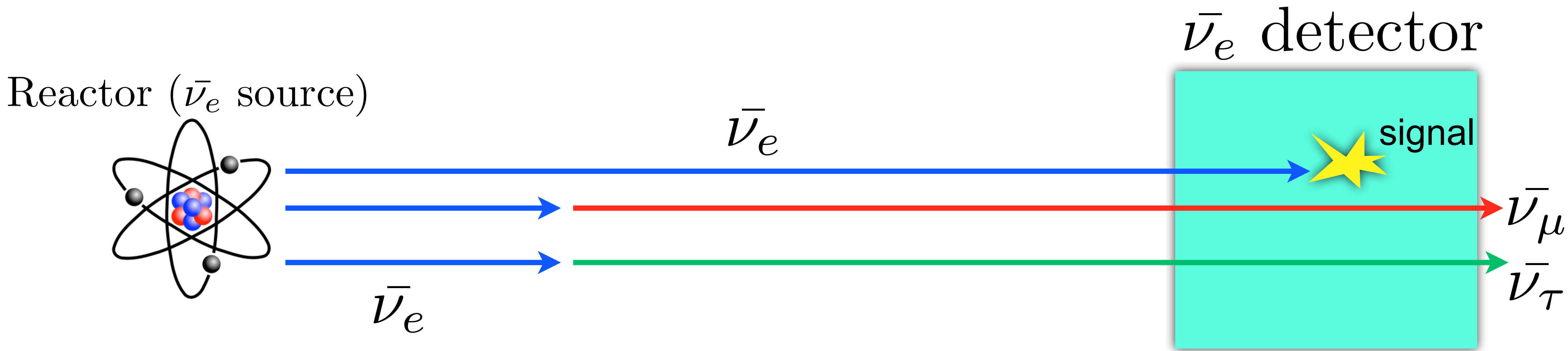
Reactor Disappearance Experiments

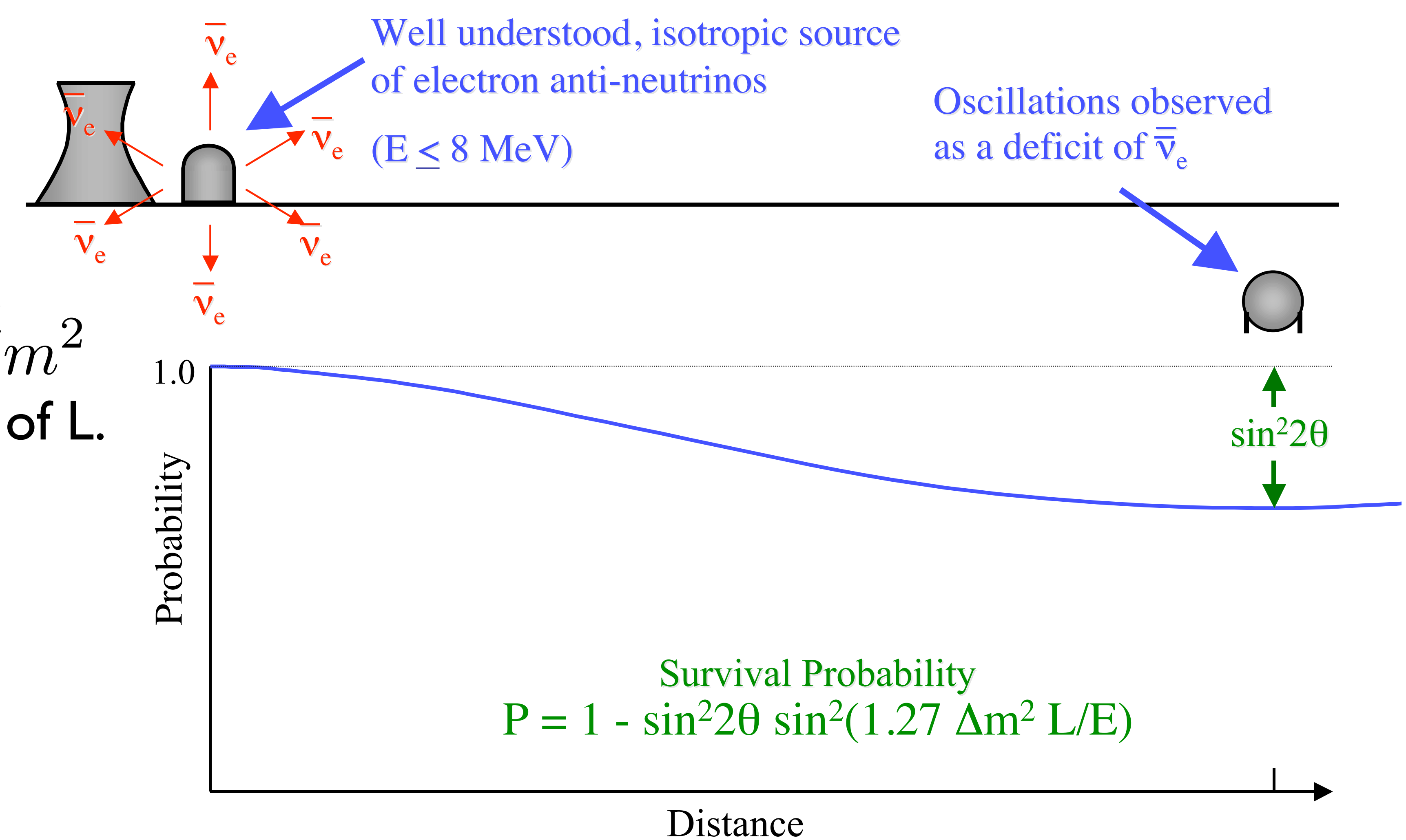


In a *disappearance experiment*, we look for a deficit of electron antineutrinos.



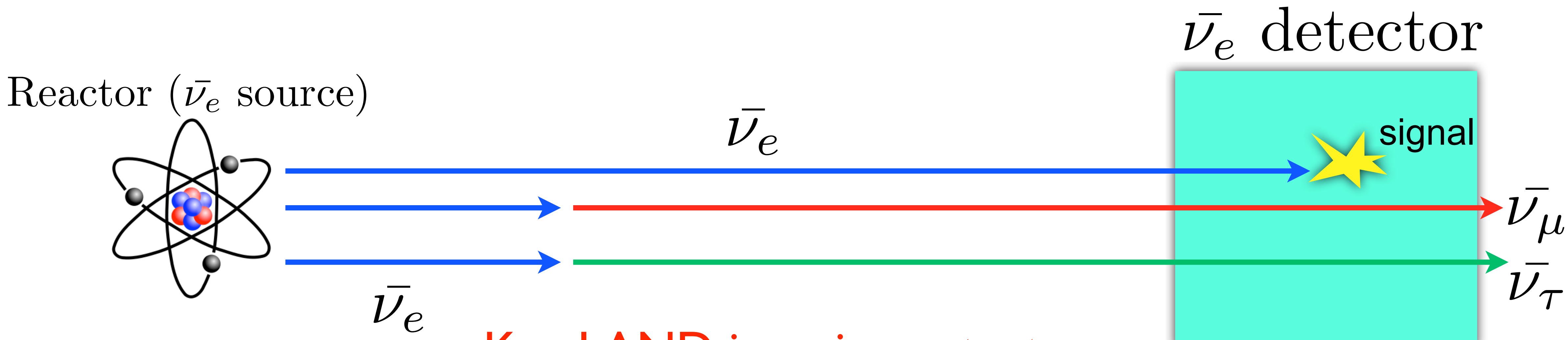
Reactor Disappearance Experiments



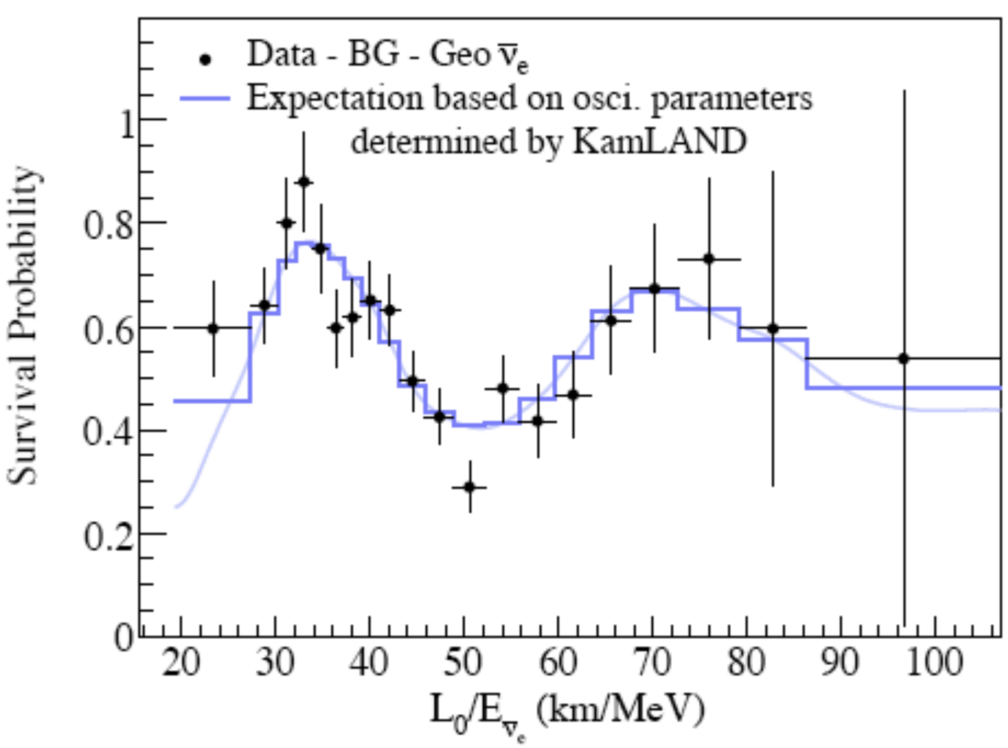


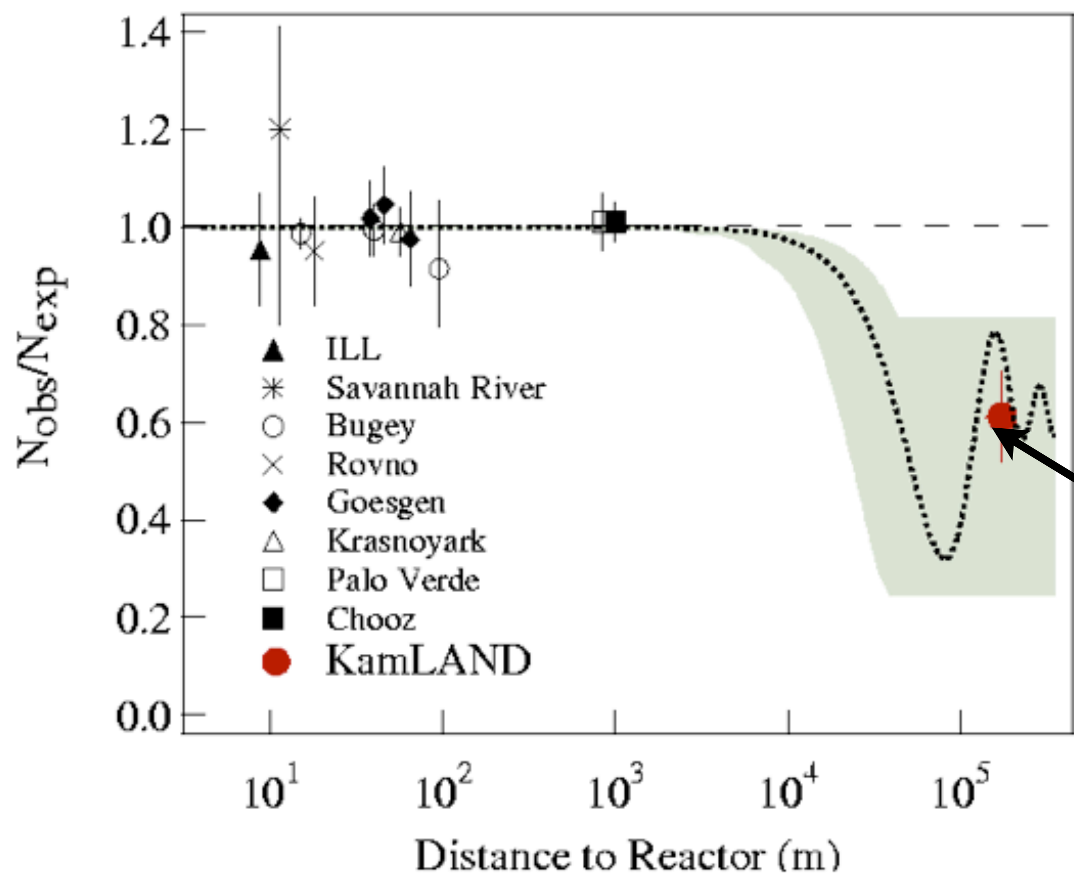
E is essentially fixed.
We can tune the δm^2
sensitivity by our choice of L.

Reactor Disappearance Experiments



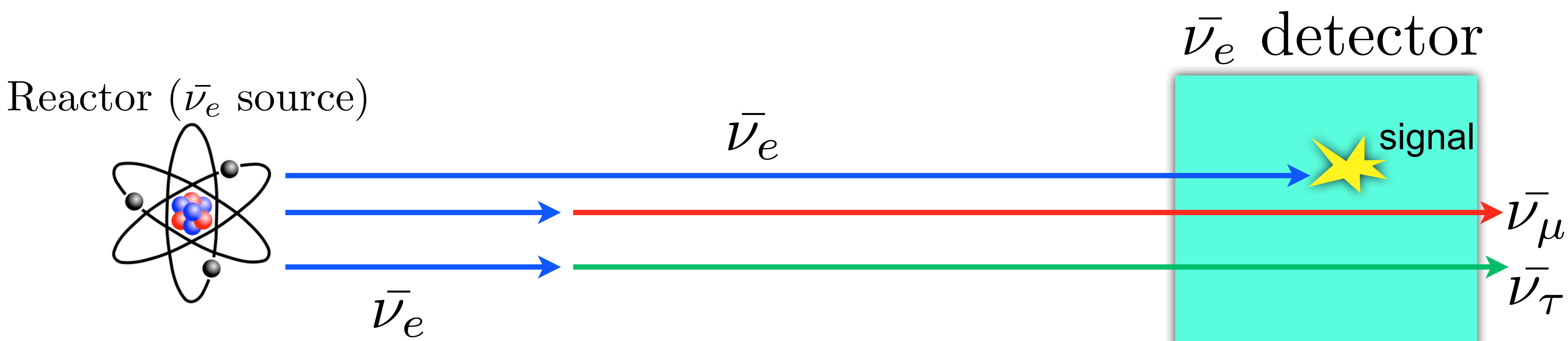
KamLAND is an important proof-of-principle.





Large L, sensitive to small δm^2 (solar)

Reactor Disappearance Experiments

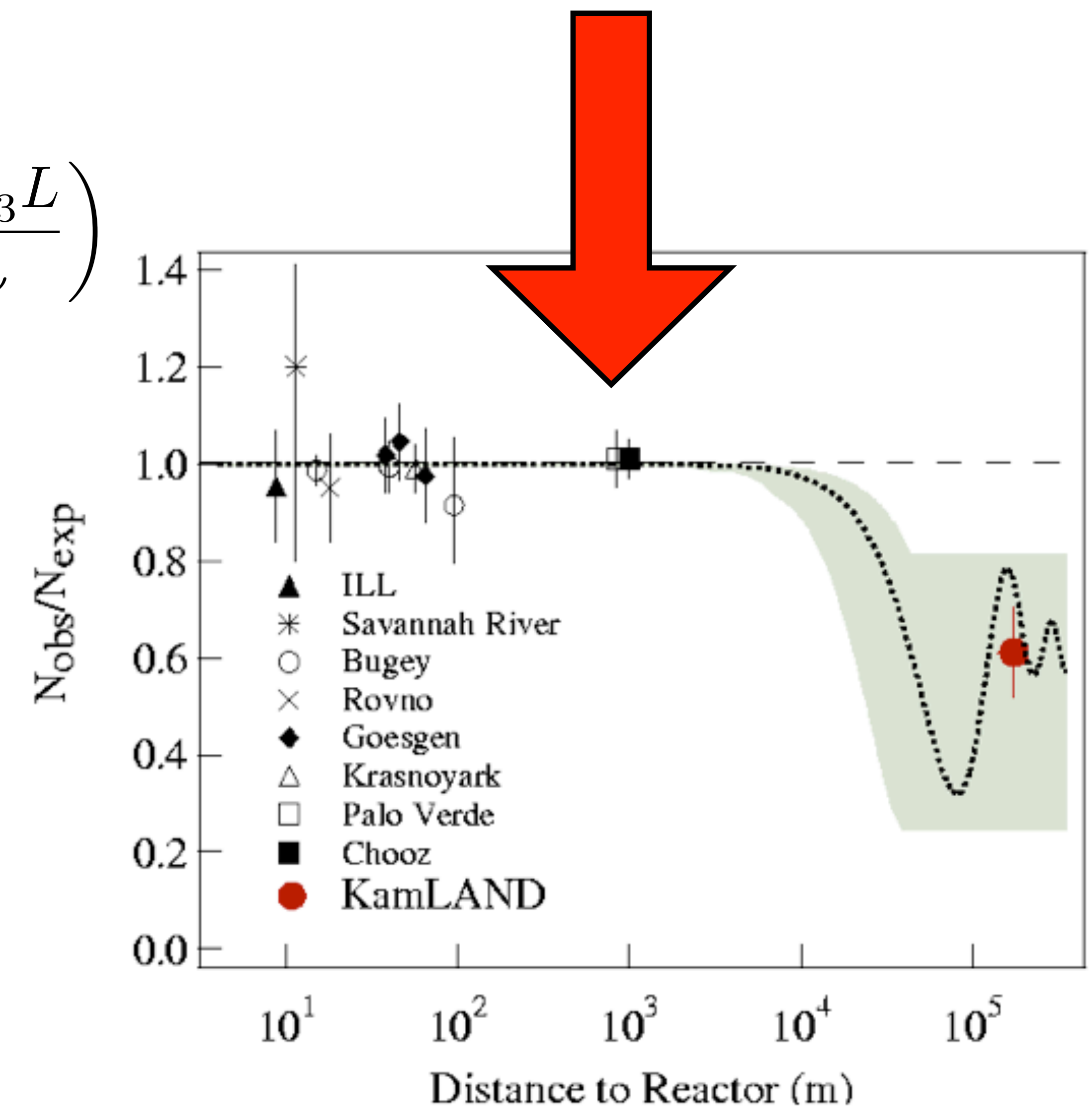


For our study, we will use $L \approx 1$ km...

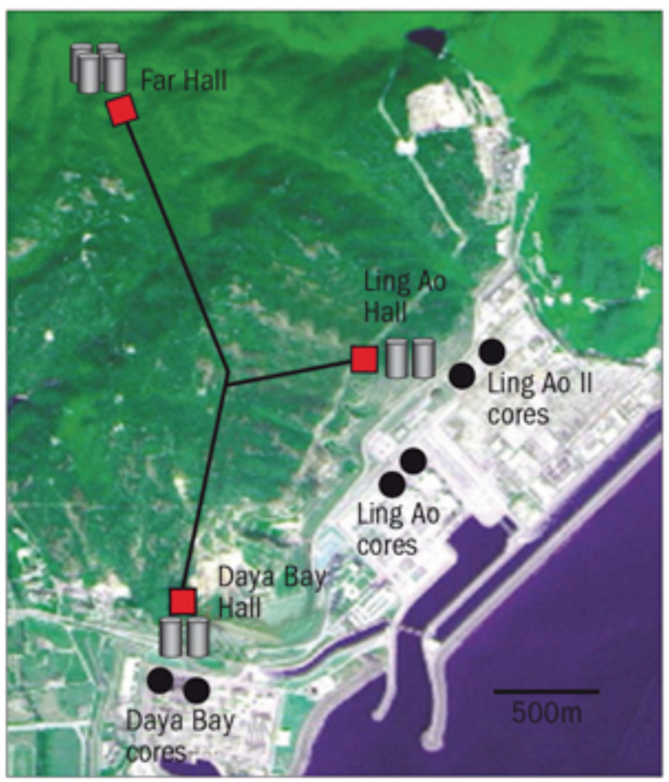
where...

$$P_{dis} \approx 1 - \sin^2 2\theta_{13} \sin^2 \left(1.27 \frac{\delta m_{13}^2 L}{E_\nu} \right)$$

We need higher precision than past experiments.



Three Reactor Neutrino Experiments



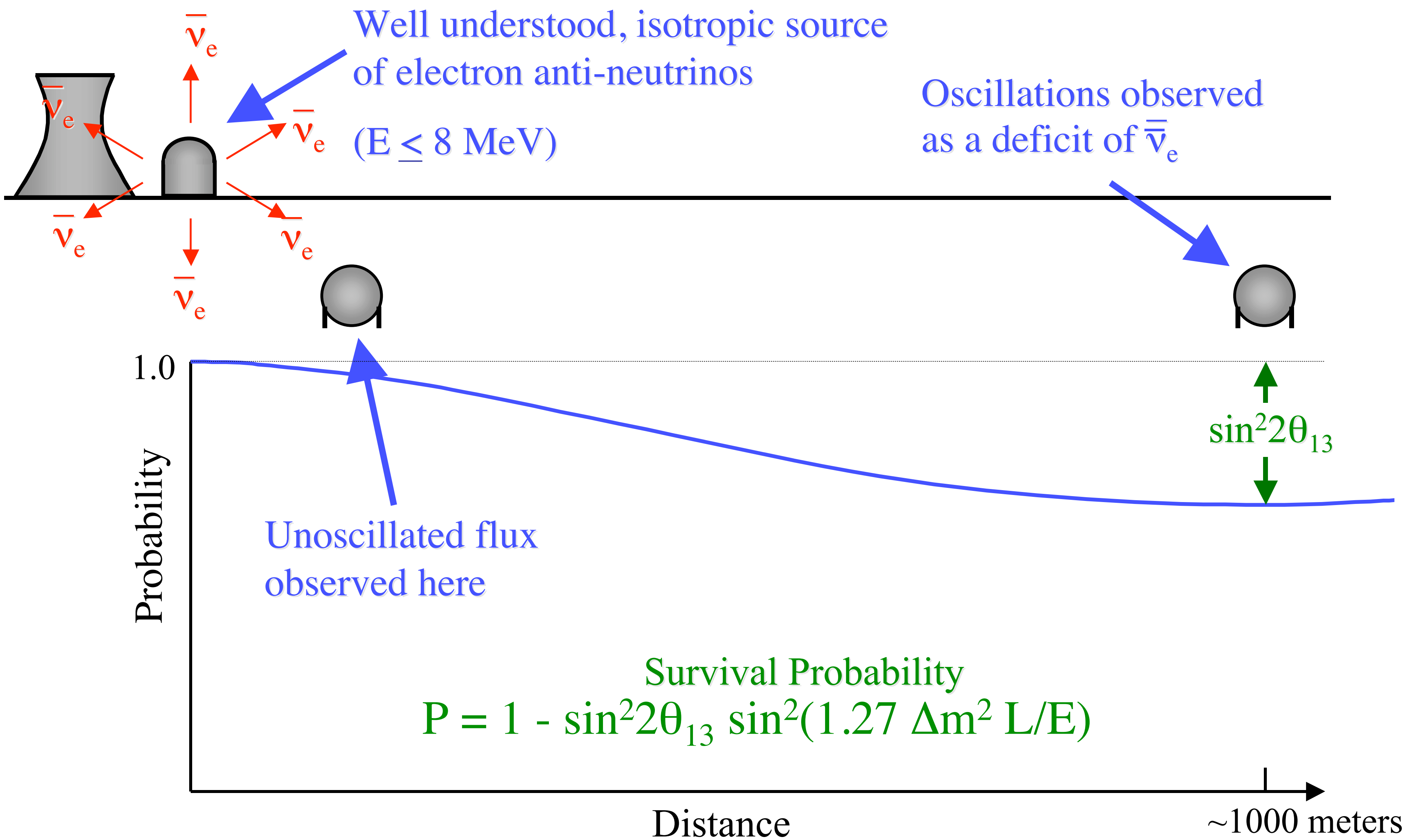
arXiv:hep-ex/0701029v1

arXiv:1003.1391v1

arXiv:hep-ex/0606025v4

All three experiments employ the same near-far detector principle.

However, unlike Daya Bay and RENO, Double Chooz will activate its near detector much later.



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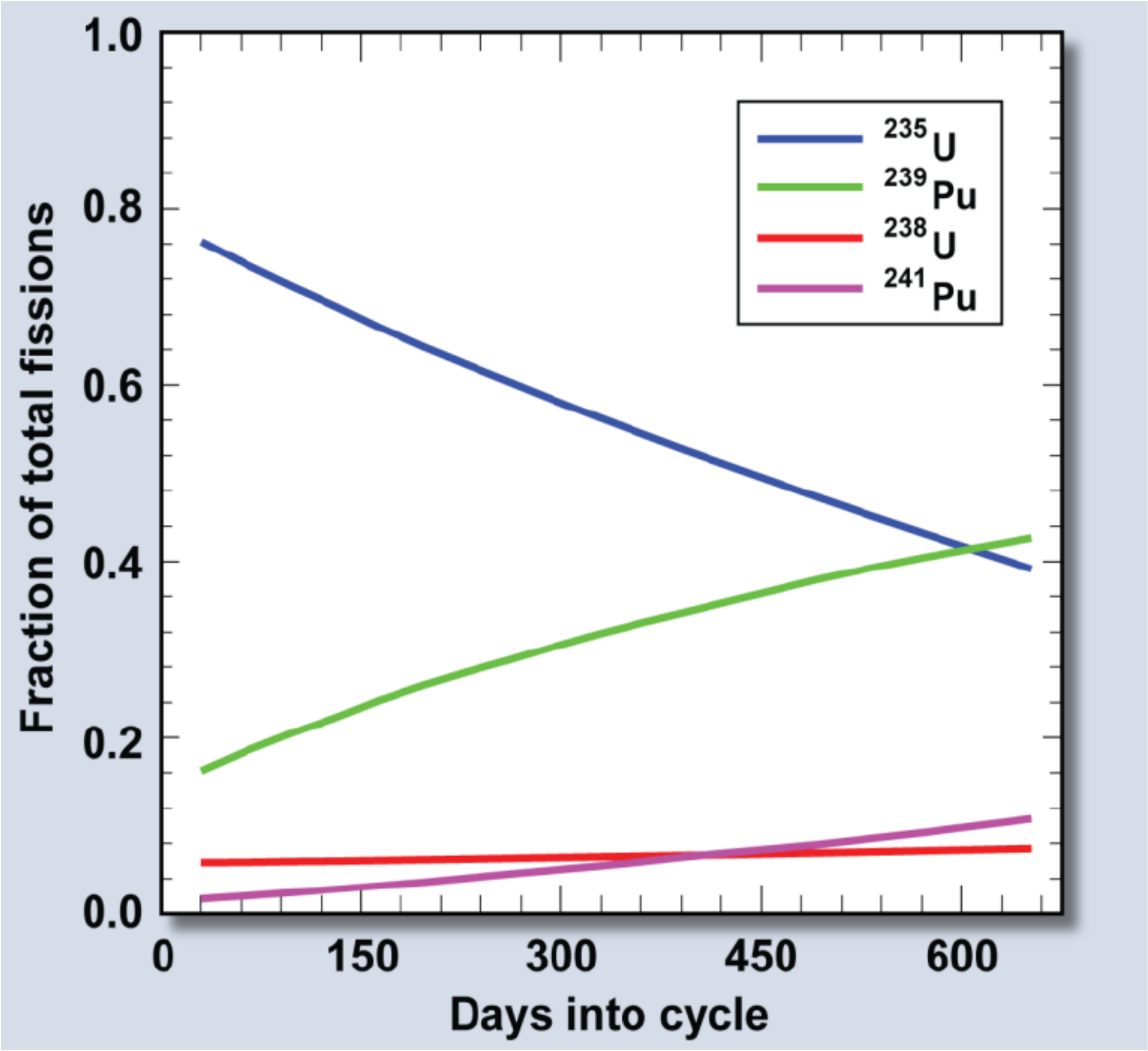
Where In the World is Chooz?

The Experiment

The 4 Most Important Fissile Nuclides



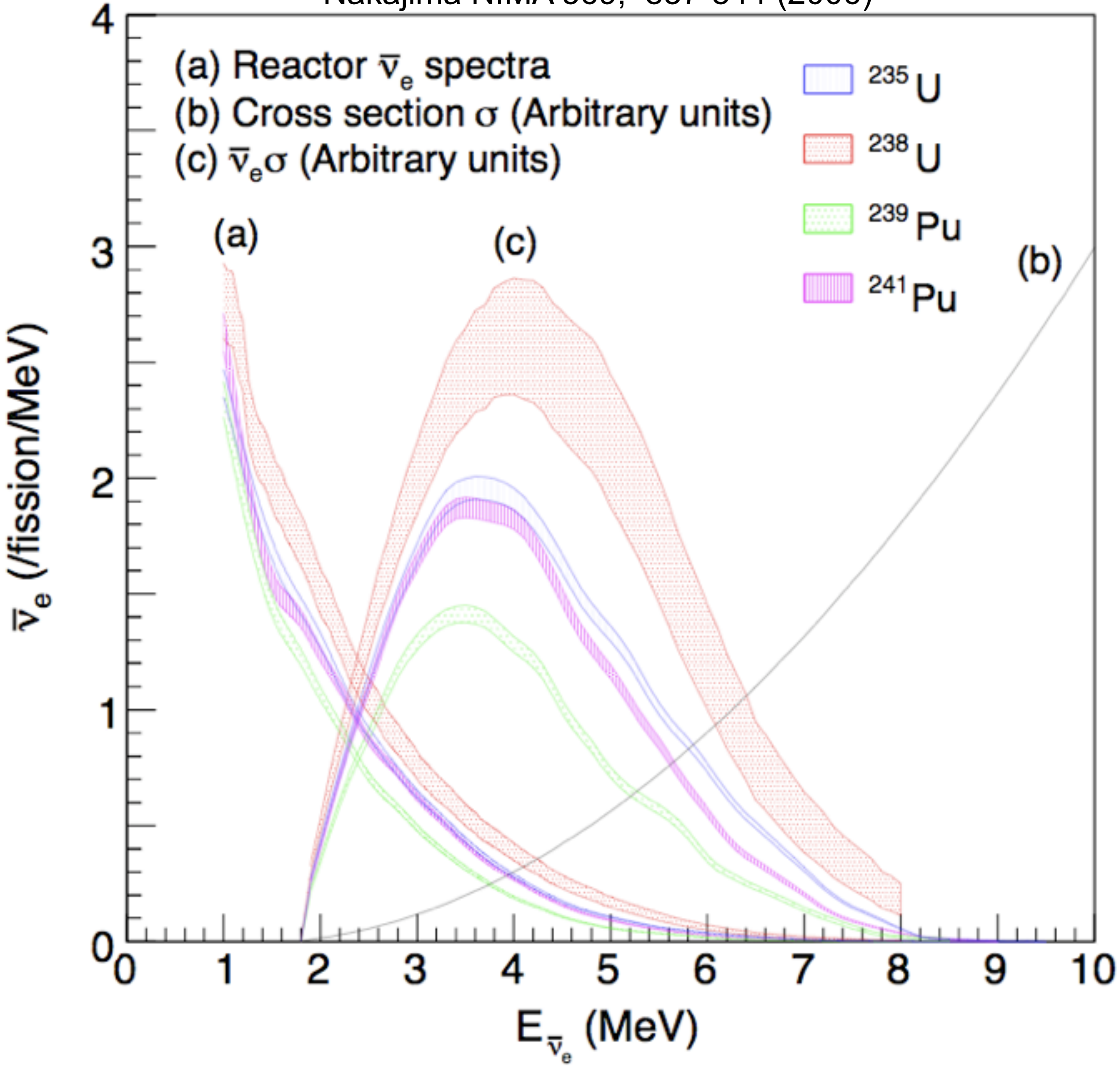
Nuclide	average % of fissions in fuel cycle
U235	55.6
Pu239	32.6
U238	7.1
Pu241	4.7

arXiv:0606025v4

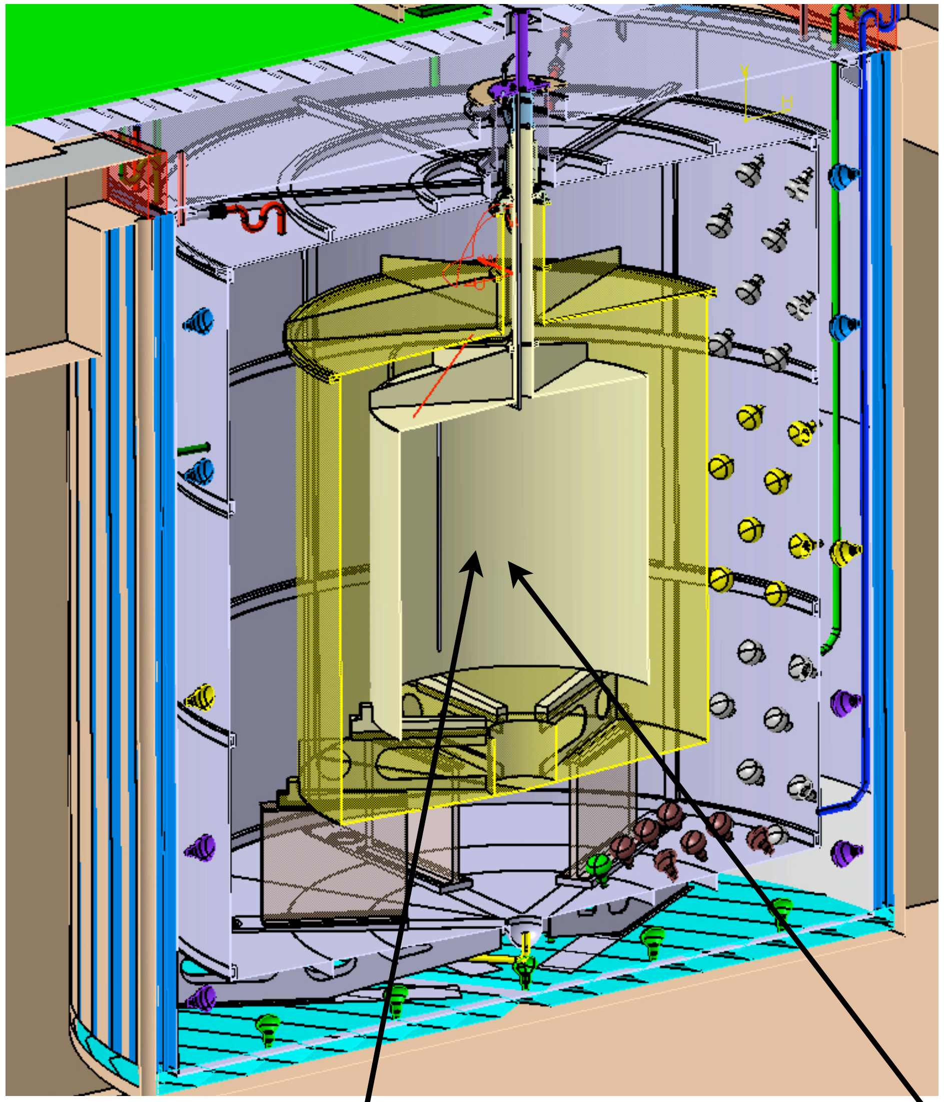
- 2×10^{20} anti-neutrinos per s per GW_{th}

All fissions are not created equal!
U and Pu spectra are different.
Our signal is enhanced by the cross section's energy dependence.

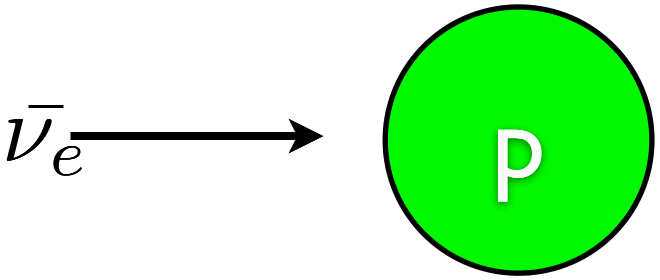
Nakajima NIMA 569, 837-844 (2006)



How We Detect Events: Inverse Beta Decay



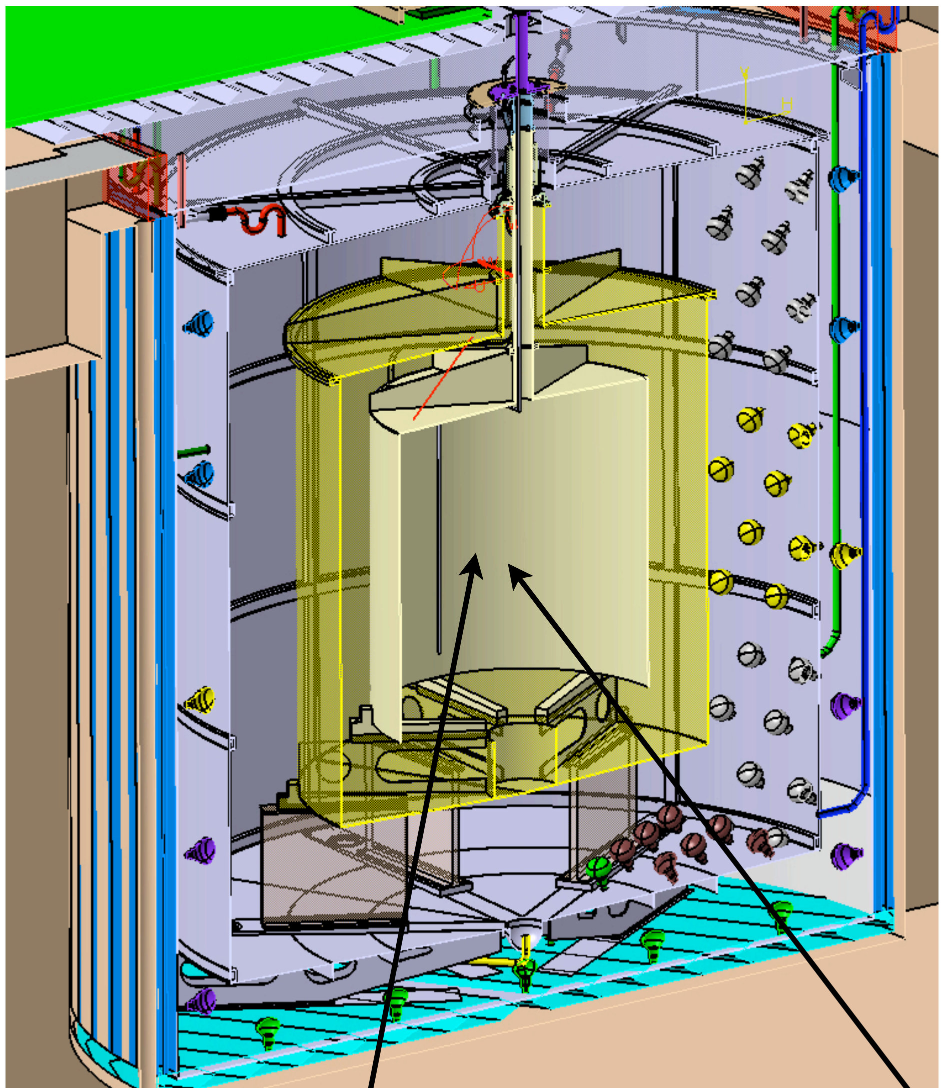
$$p + \bar{\nu} \rightarrow n + e^{+}$$



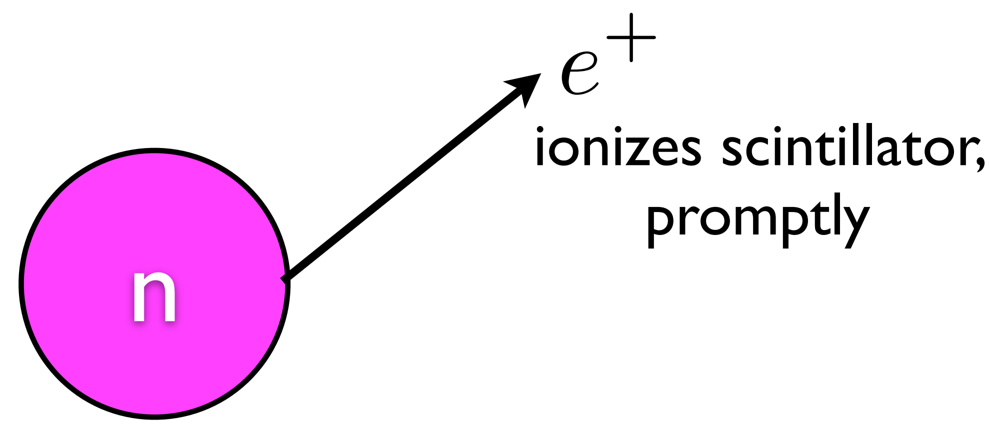
Oil provides our free protons

Gadolinium enhances our neutron capture

How We Detect Events: Inverse Beta Decay



$$p + \bar{\nu} \rightarrow n + e^+$$



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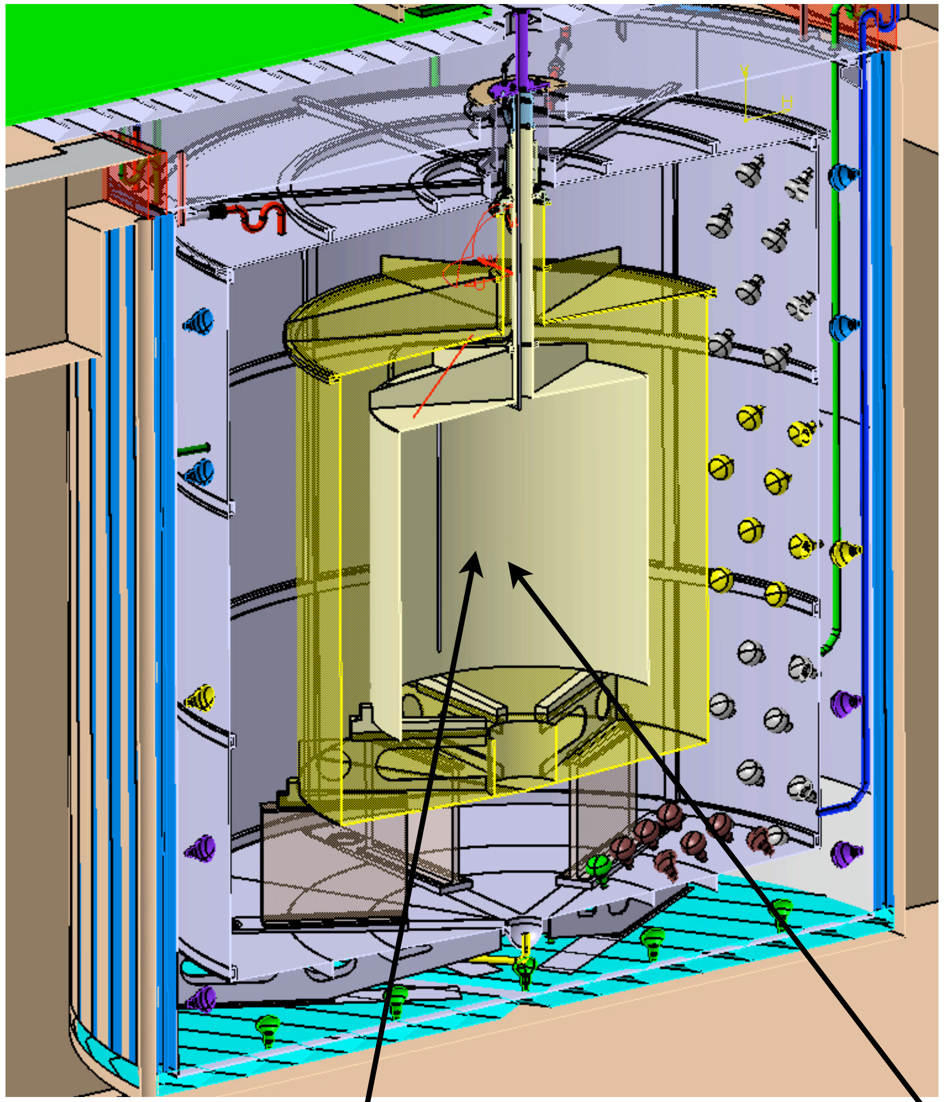
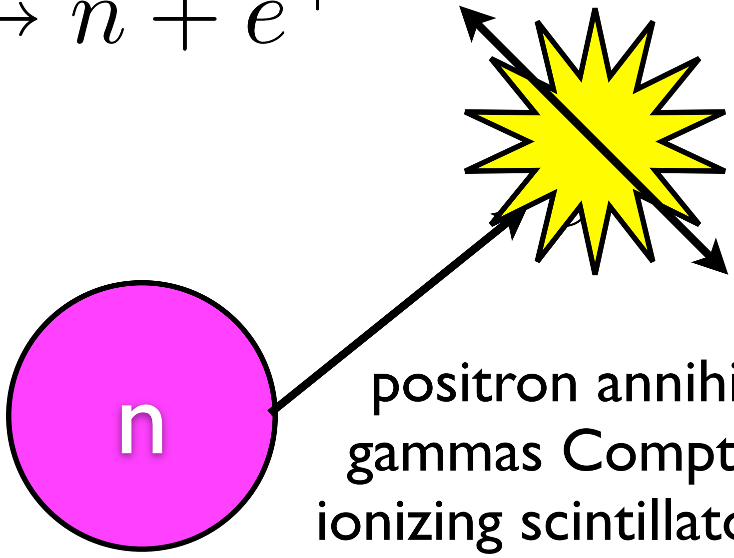


$$p + \bar{\nu} \rightarrow n + e^{+}$$

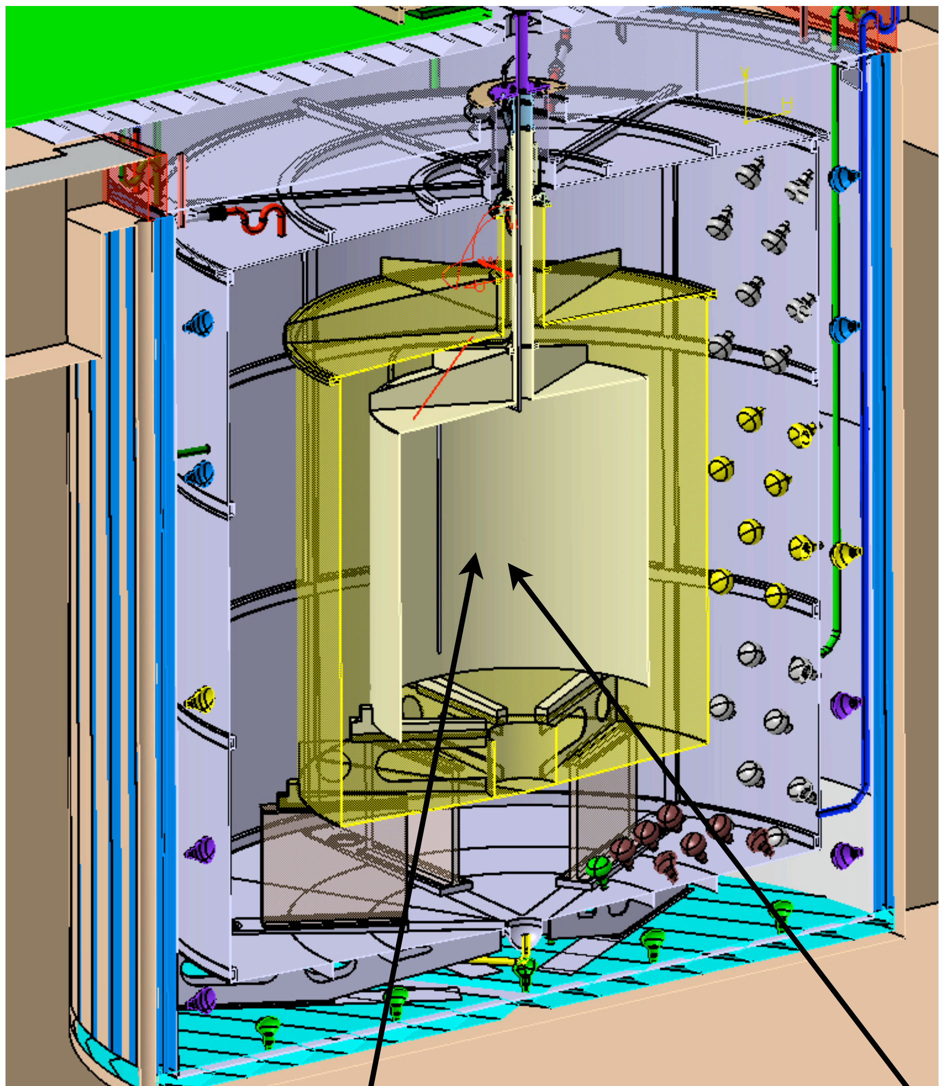


positron annihilates, and gammas Compton scatter, ionizing scintillator, all within prompt event

Oil provides our free protons

Gadolinium enhances our neutron capture

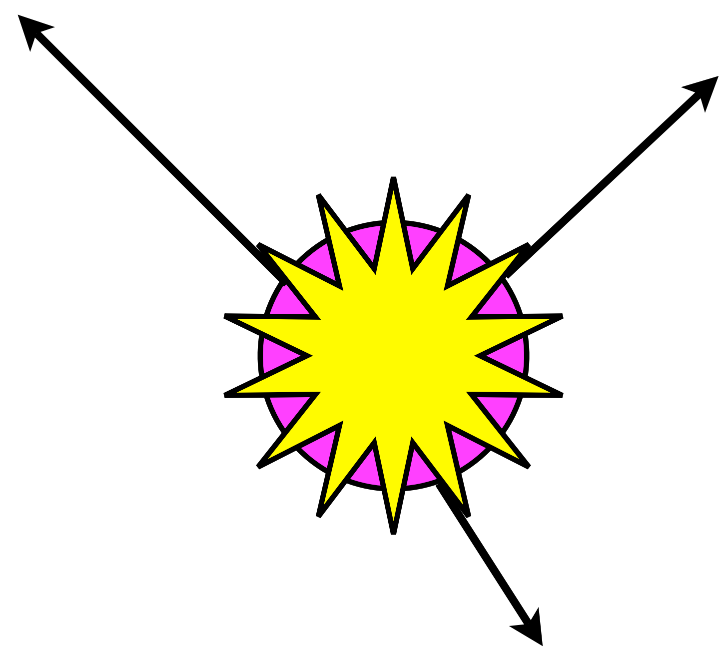
How We Detect Events: Inverse Beta Decay



$$p + \bar{\nu} \rightarrow n + e^{+}$$

About 30 microseconds later...

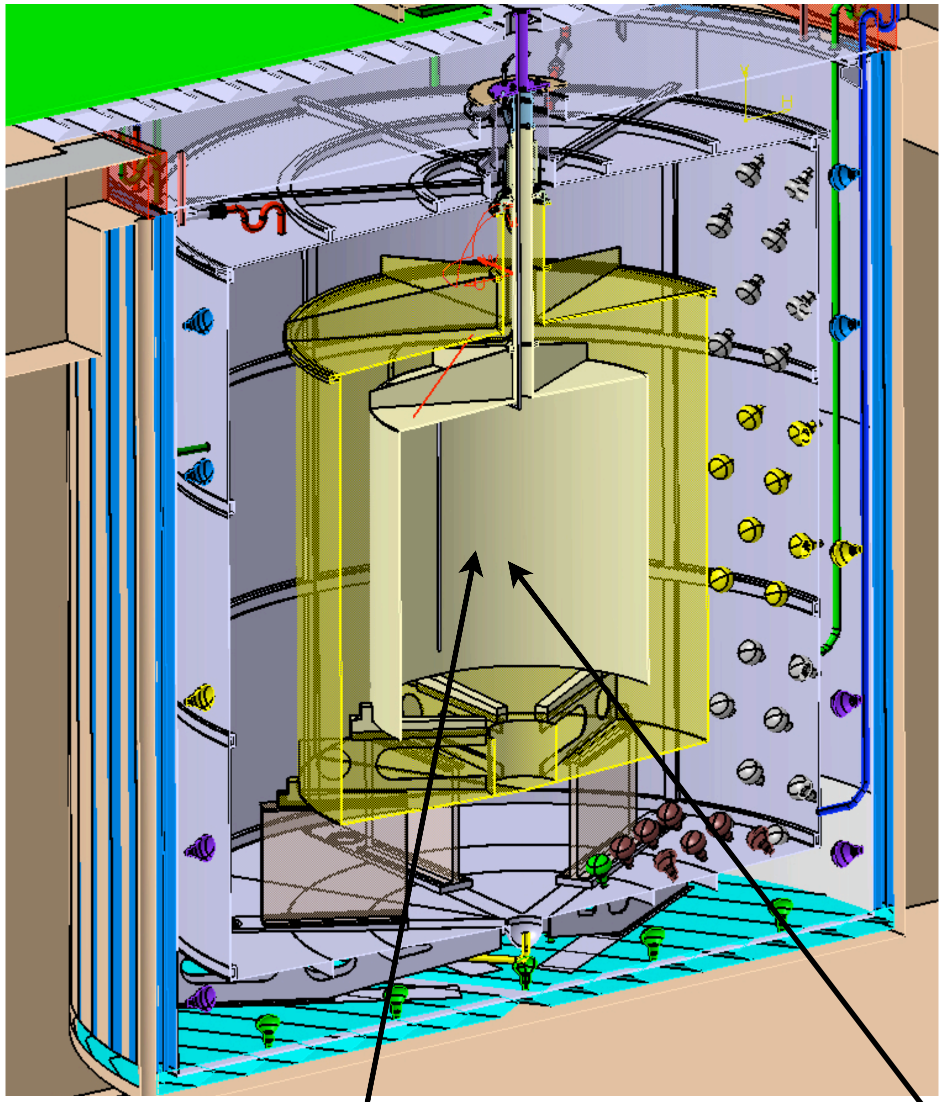
neutron captures on Gd, producing gammas which Compton scatter (delayed event)



Oil provides our free protons

Gadolinium enhances our neutron capture

How We Detect Events: Inverse Beta Decay



$$p + \bar{\nu} \rightarrow n + e^{+}$$

Prompt

Delayed

A coincidence signal!

Oil provides our free protons

Gadolinium enhances our neutron capture

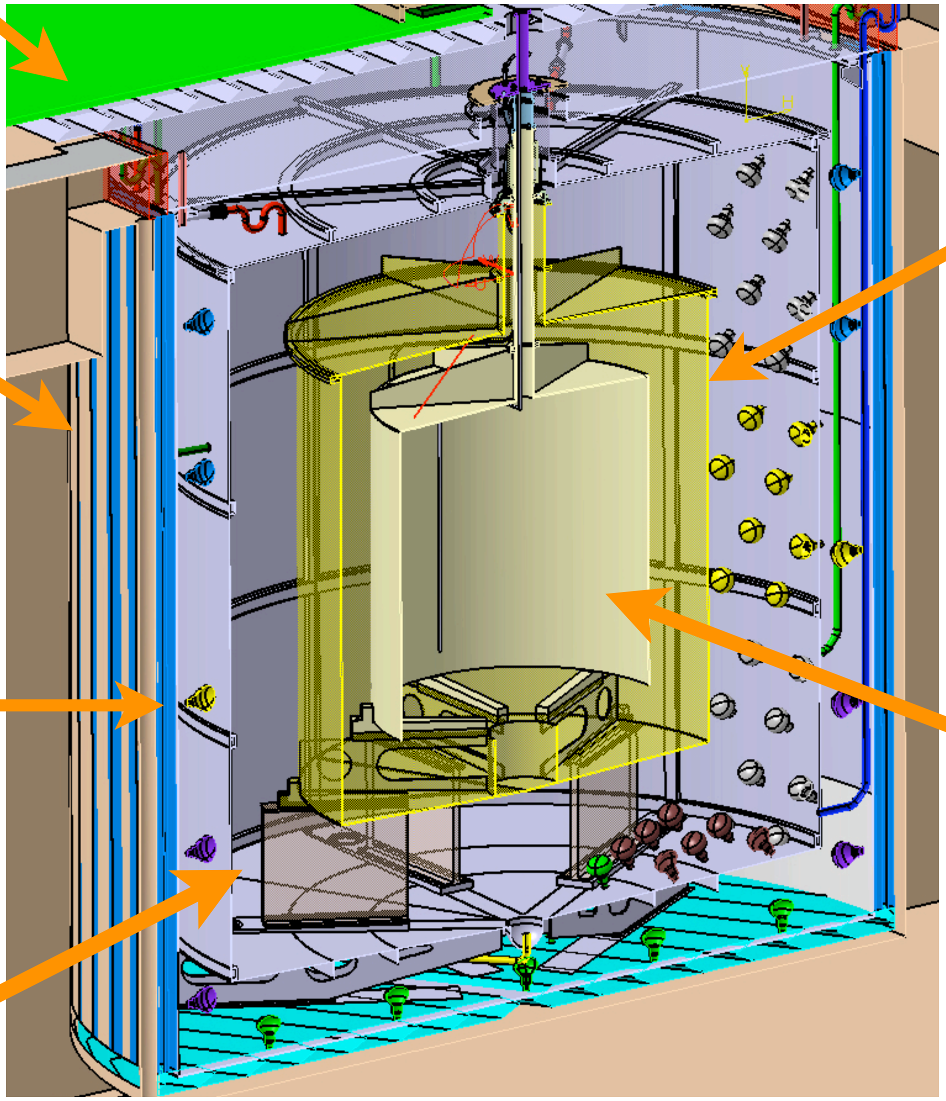
Double Chooz Detector

Outer Veto

Shielding

Inner Veto
(90m^3 LAB LS)

Buffer
(110m^3 Mineral Oil)



Gamma Catcher
(22.6 m^3 LS)

Target
(10.3m^3 Gd doped LS)

Other θ_{13} experiments use similar designs.

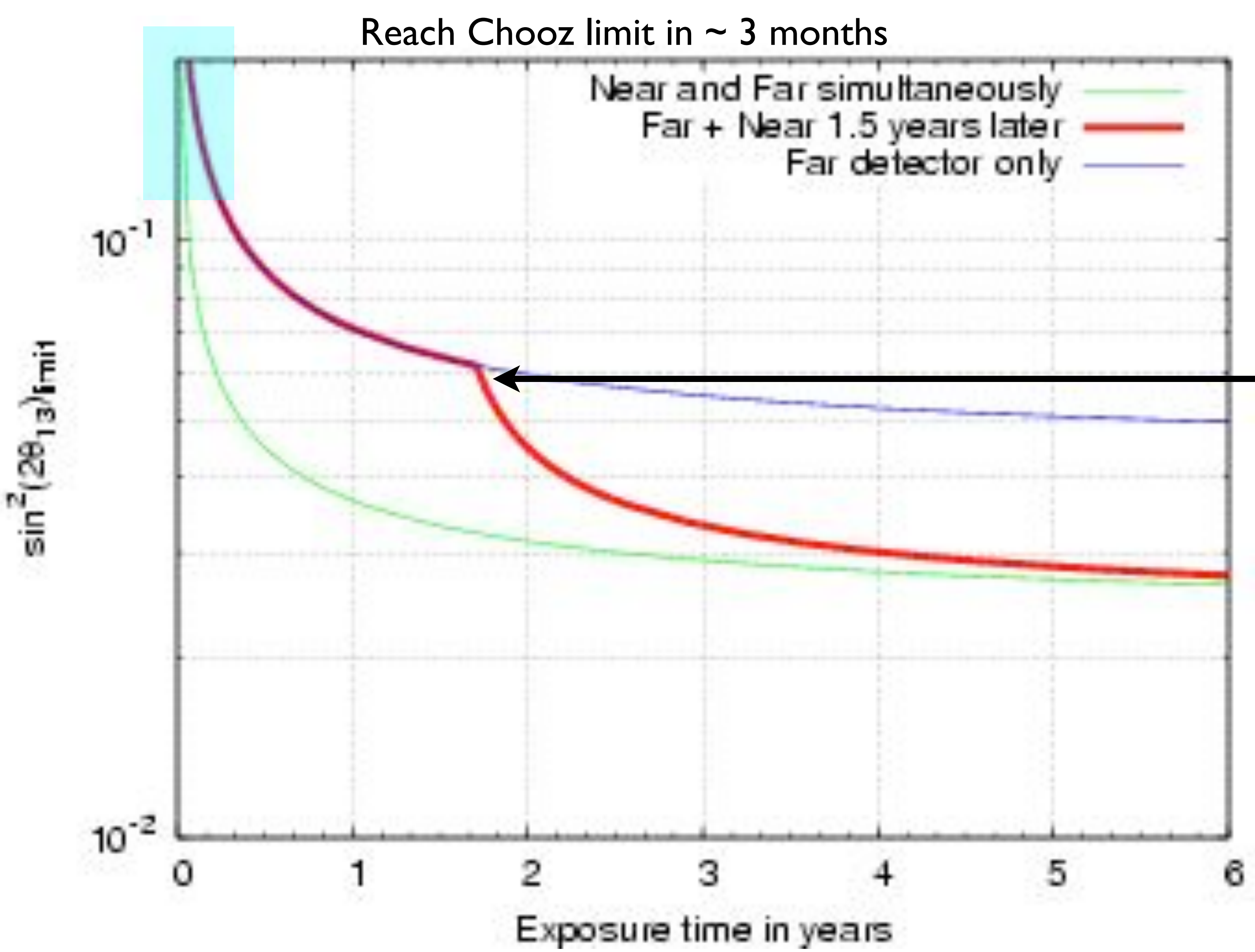
Summary for Past versus Present Designs

Improvements come from...

1) Improved detector design

2) Near-far combination

But, Double Chooz is building its detectors sequentially...



Until Near Detector is activated, sensitivity is limited by prediction of reactor flux!

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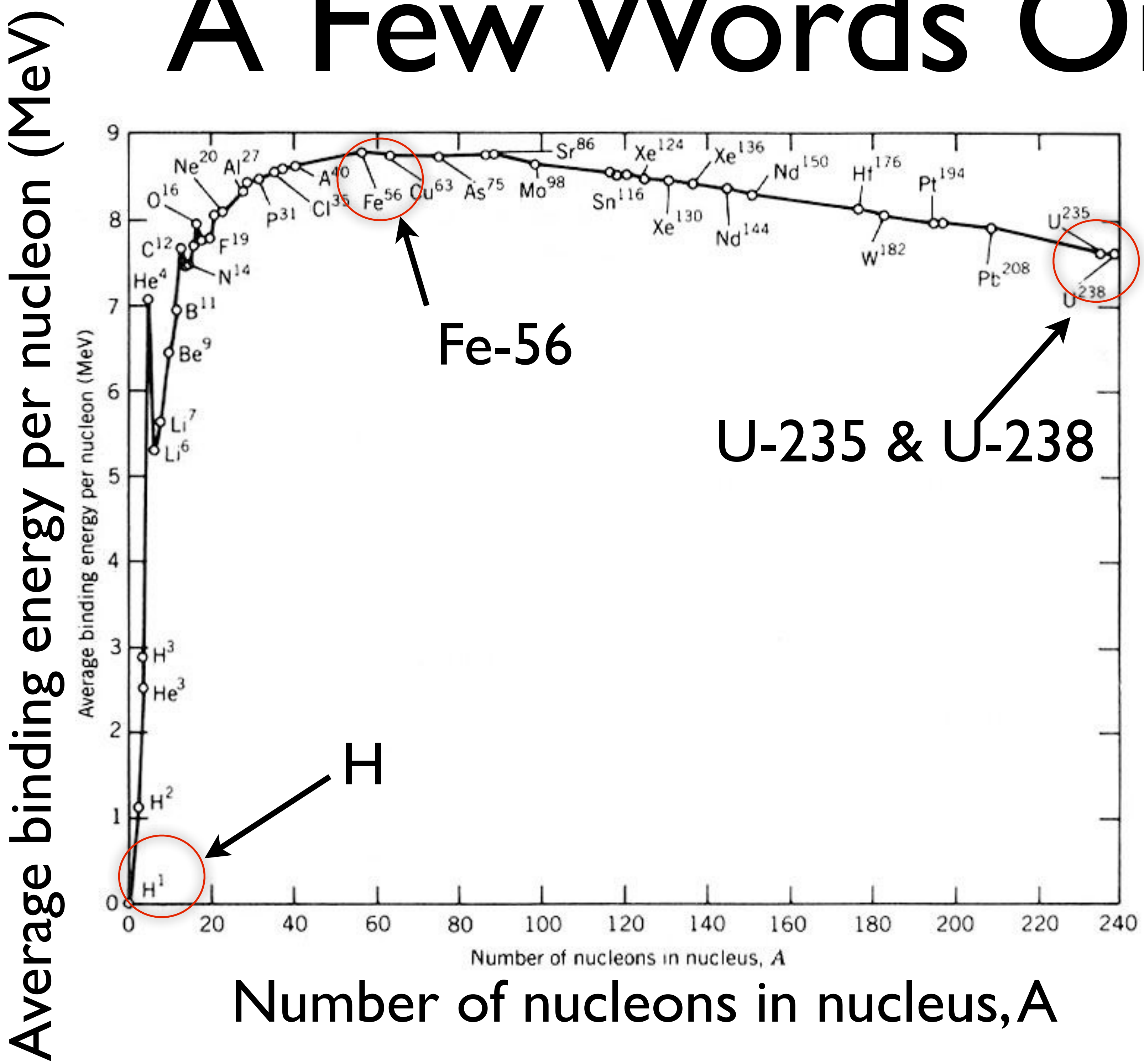
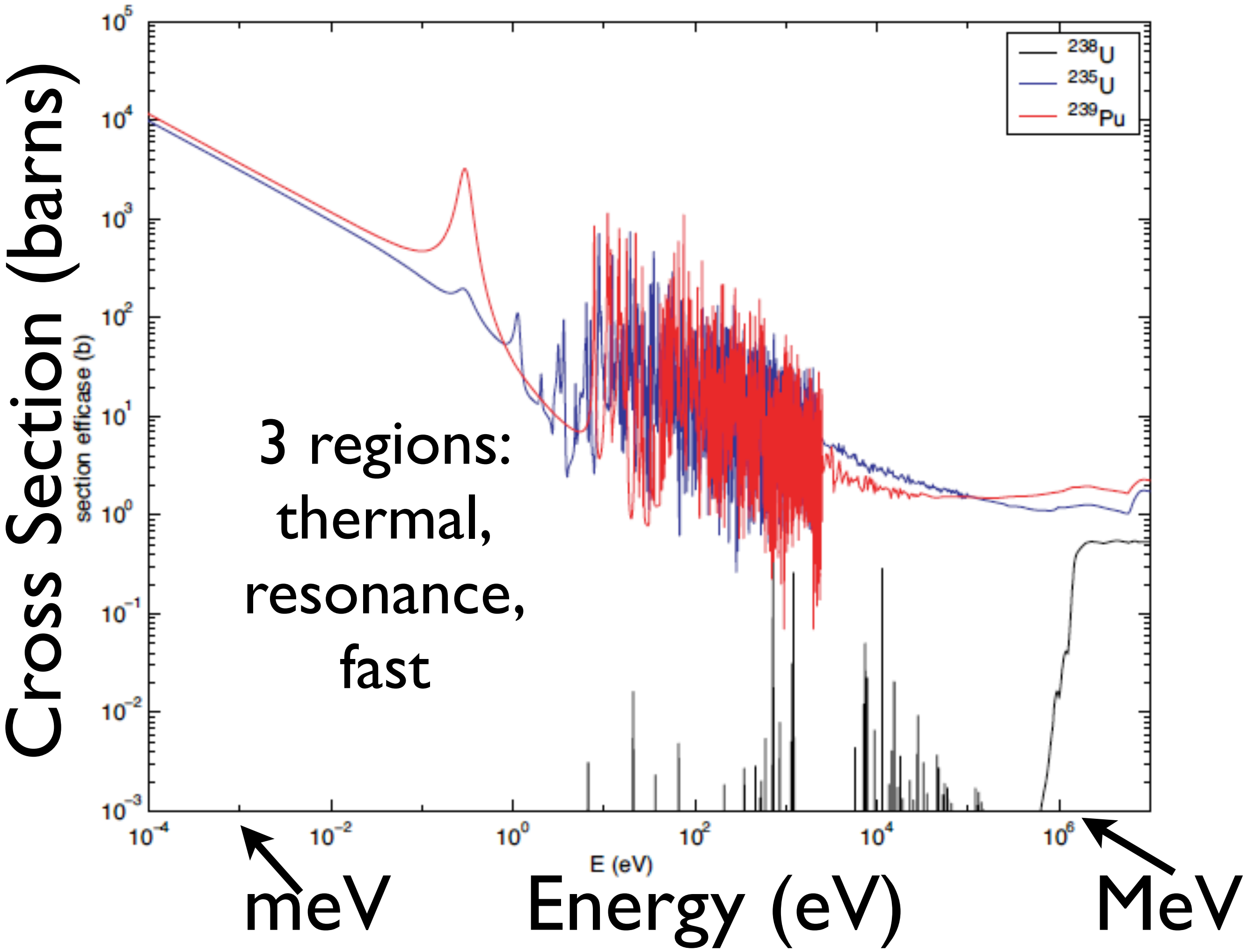
A Few Words On Fission

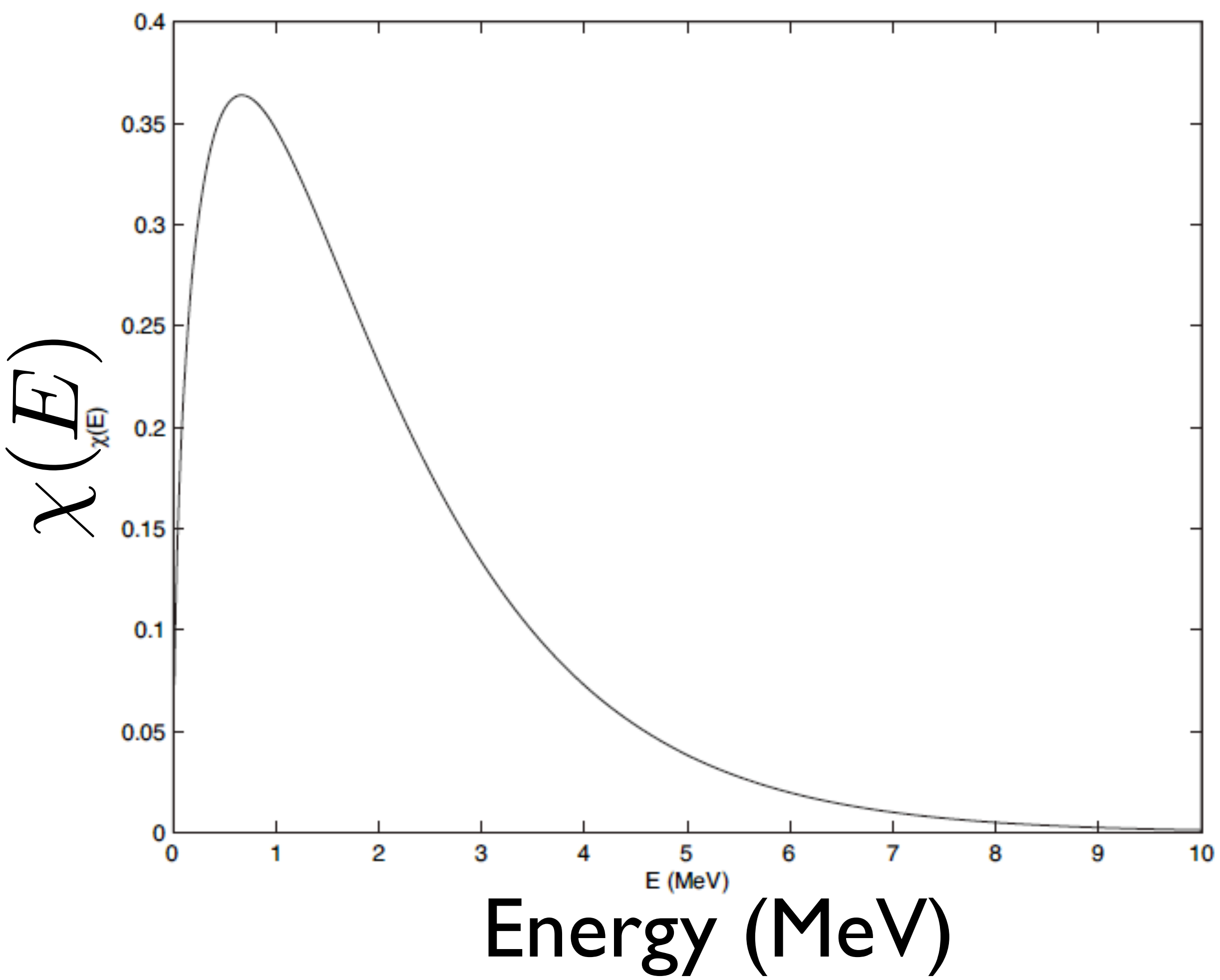


- Heavy isotopes are *fissile* if slow (thermal) neutrons cause fissions

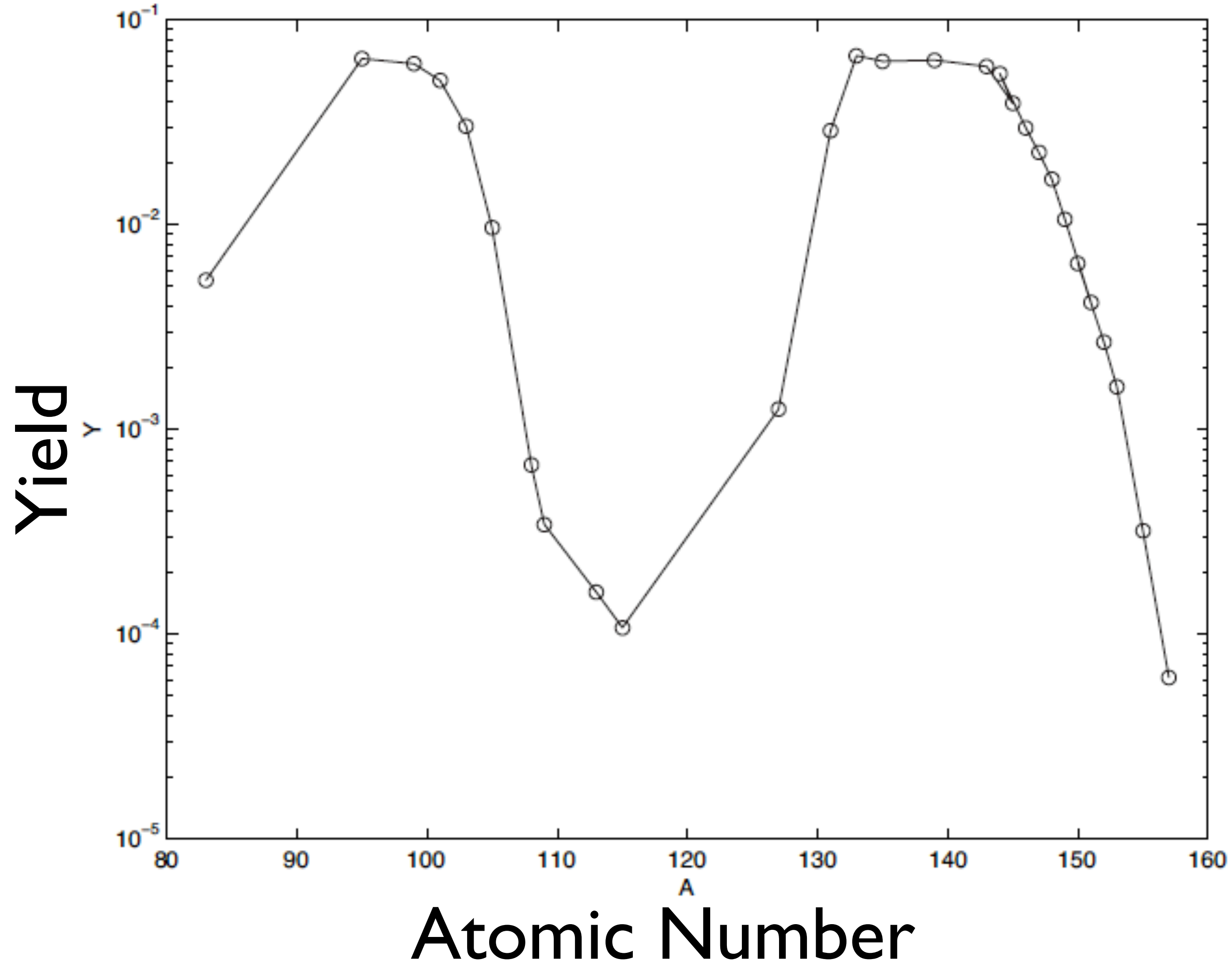


Fission Cross Sections

Neutron Energy Probability Distribution



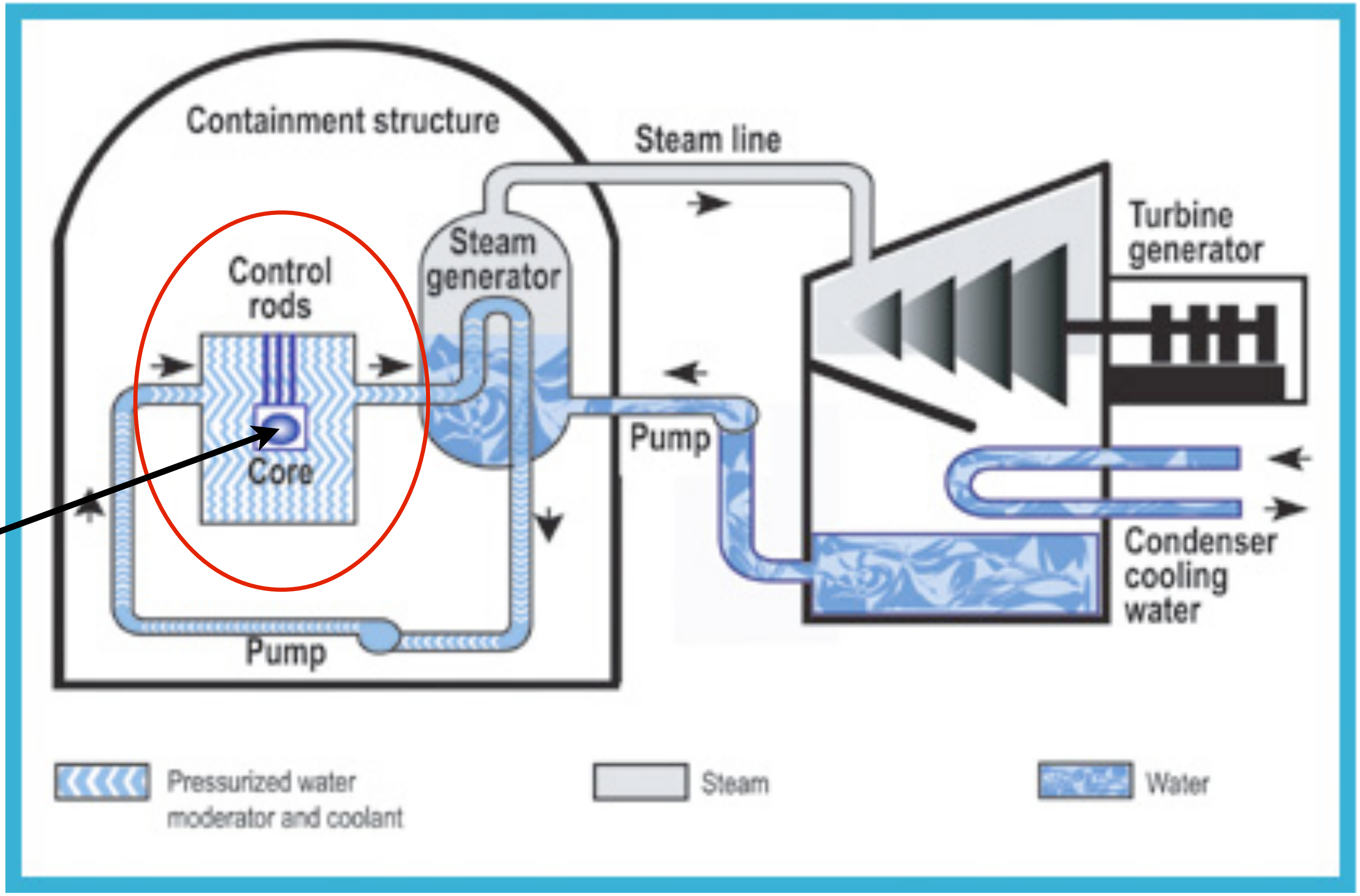
Fission Yield for Uranium-235



$6\bar{\nu}_e$ produced on average per fission

$$^{235}_{92}U + n \rightarrow^{94}_{40} Zr +^{140}_{58} Ce + 2n$$

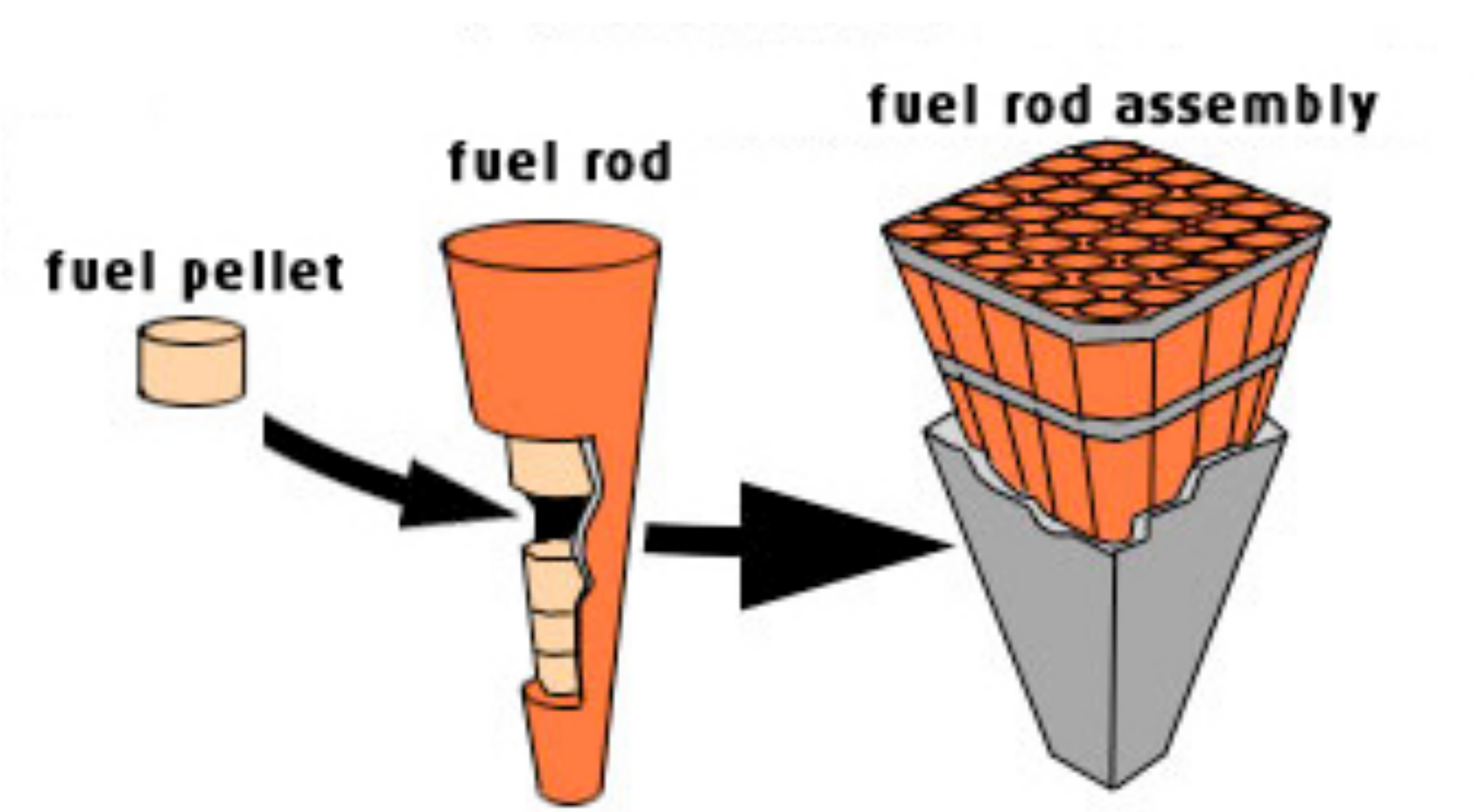
How A Nuclear Reactor Works



We'll be focusing on this part only!

Reactors, Inside Out

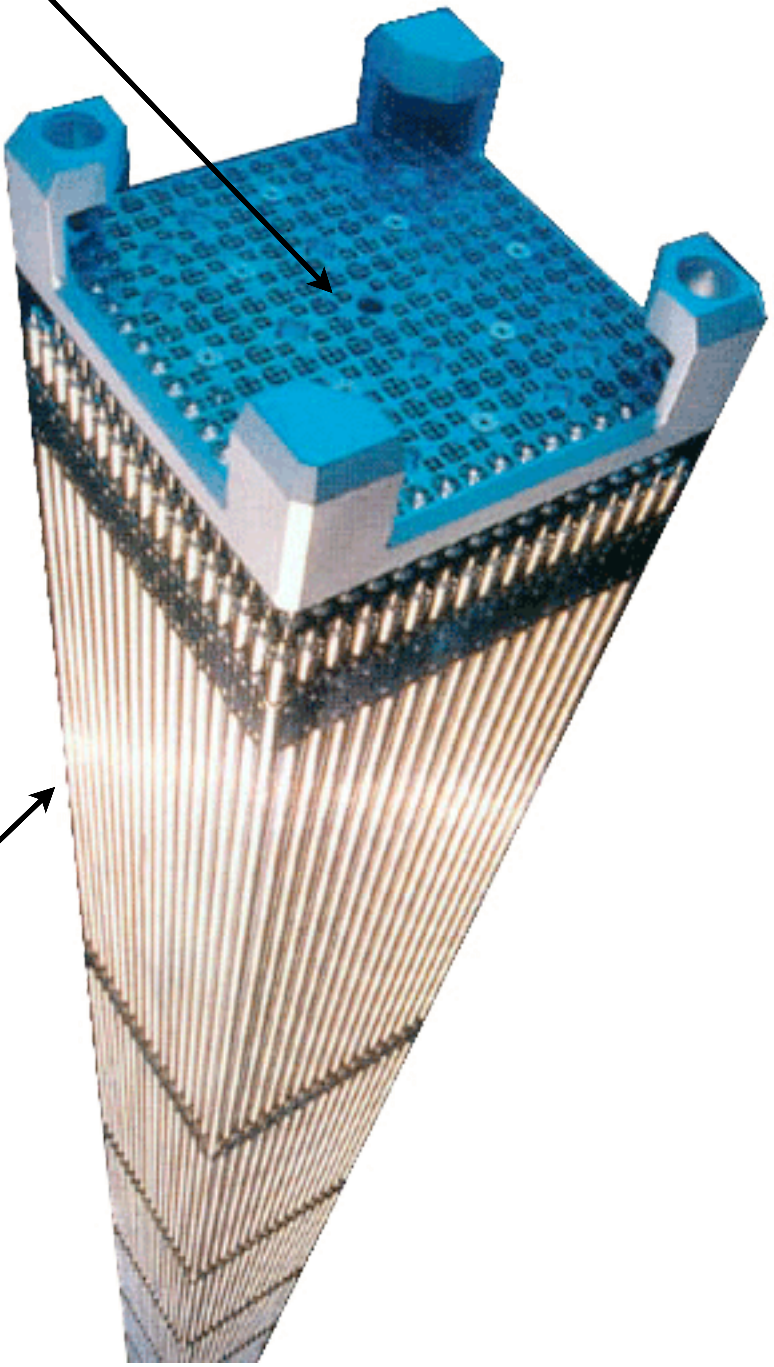
~1 cm ~400 cm



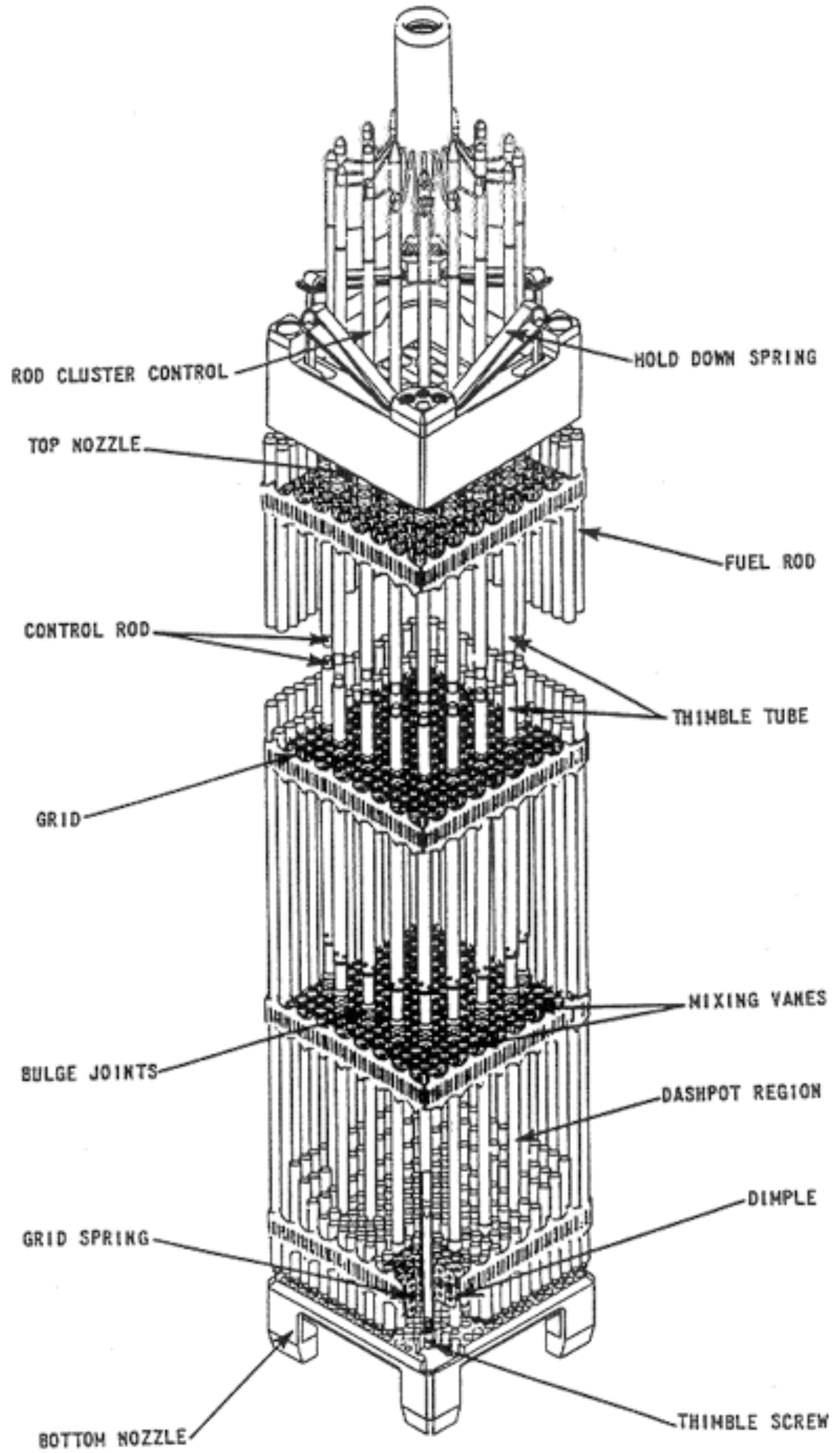
- The Chooz N4 reactors are PWRs (pressurized water reactors)
- Uranium is loaded into Zircaloy (mostly zirconium) fuel rods

Fuel Rod to Assembly
(what we need to simulate)

17 by 17 grid of fuel & control rods

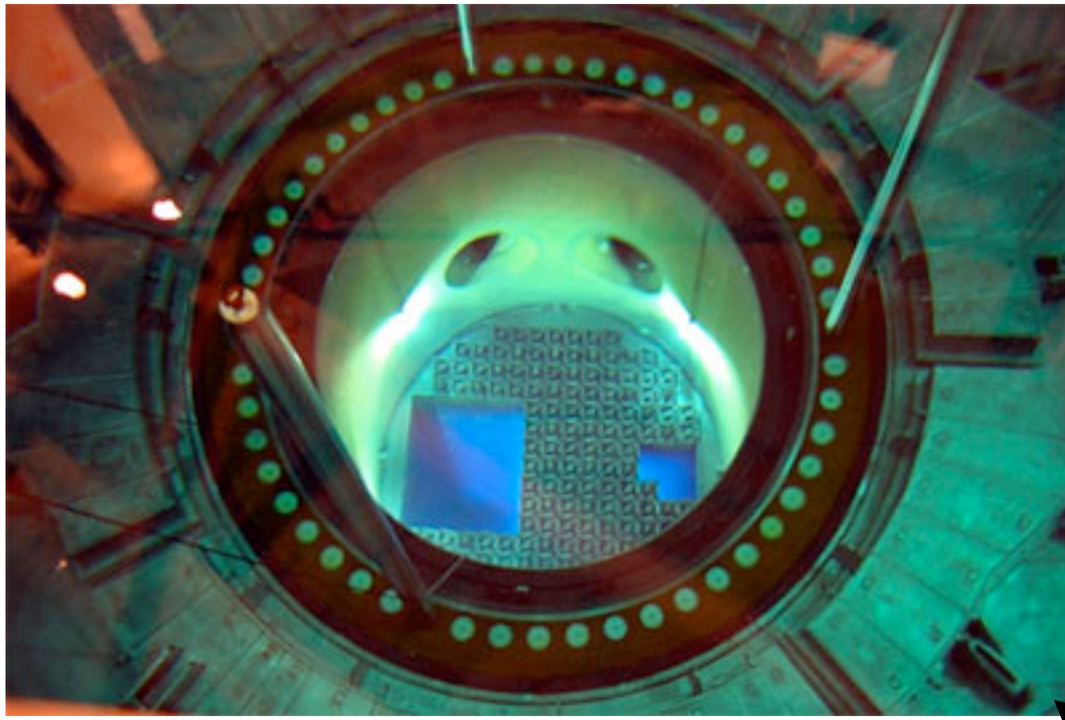


~4 m long



Reactor Fuel Assembly

From Assembly to Core

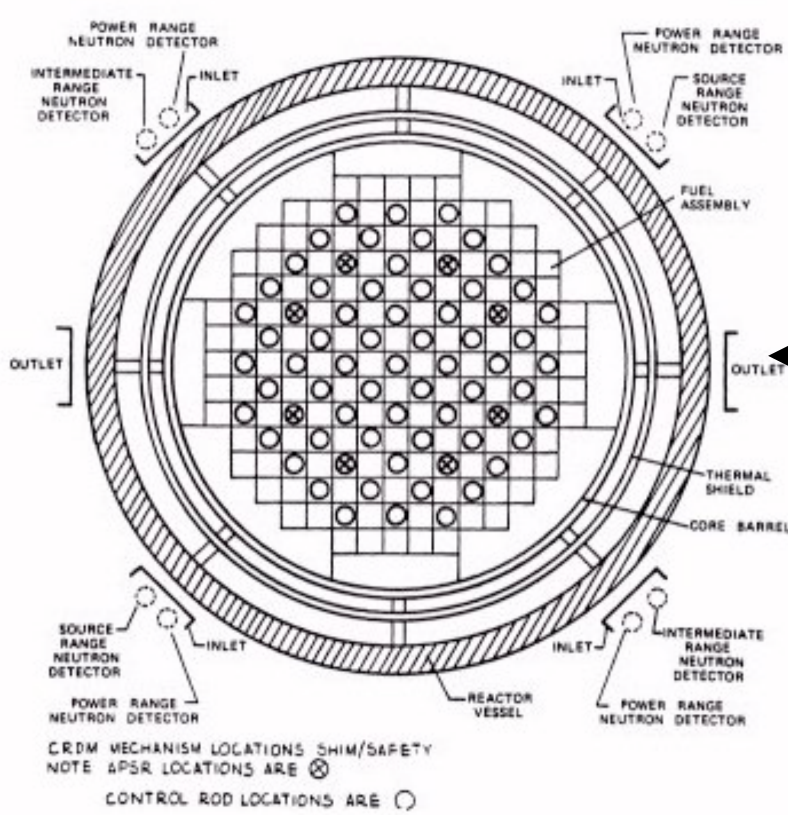


Assembly being loaded into core in Texas

eia.doe.gov

One of 19 Exelon reactors

FIGURE-4 TOP VIEW OF REACTOR CORE



Three Mile Island Core

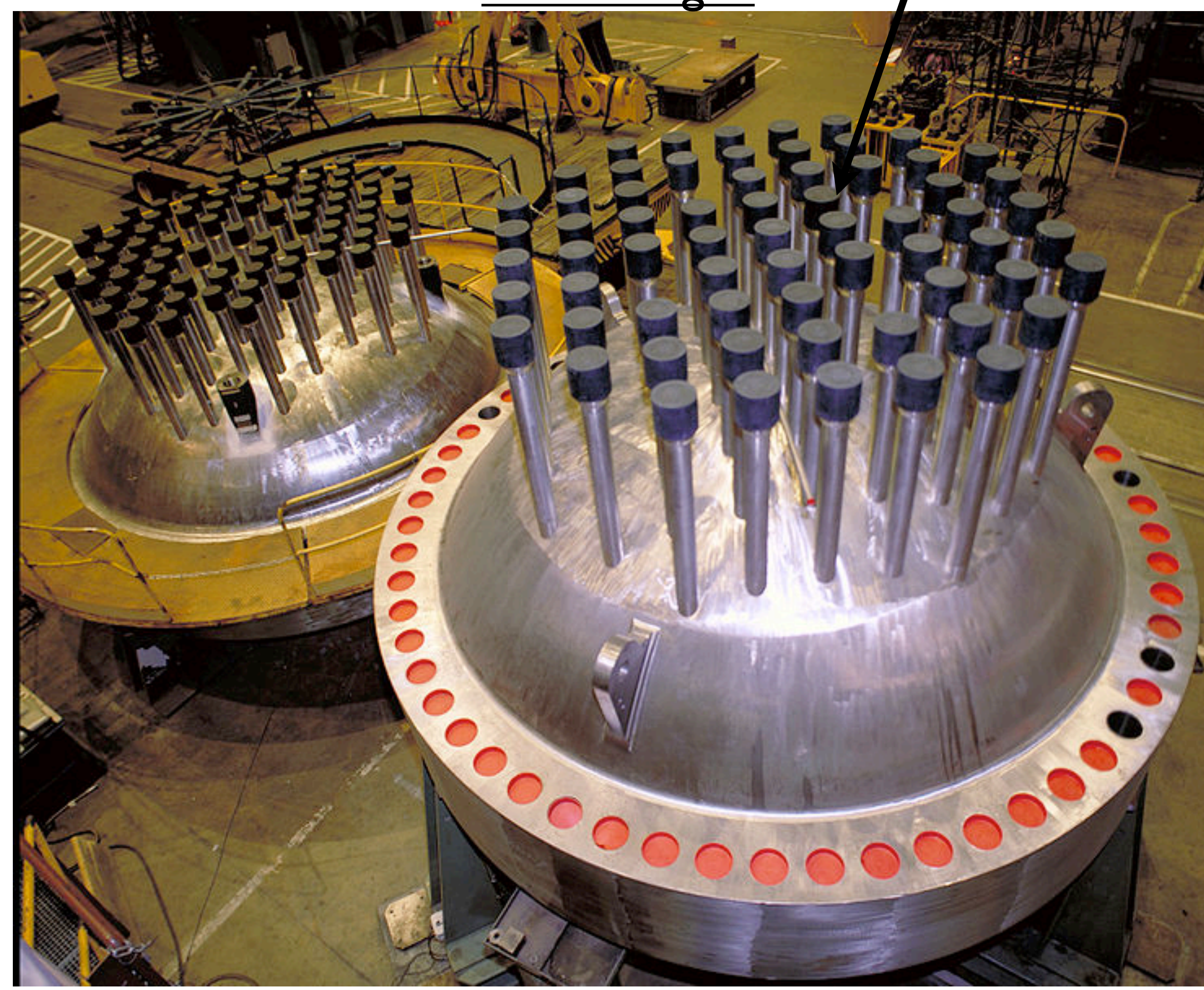
N4 reactors have 205 assemblies

http://kd4dcy.net/tmi/core.html

From Core to Vessel

Control rods

www.nrc.gov

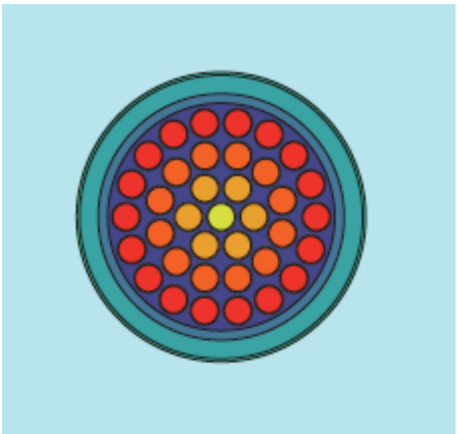


Pressurized reactor head covers core

DRAGON Basics

http://www.polymtl.ca/nucleaire/DRAGON/en/index.php

- Deterministic lattice code that calculates neutron flux in an assembly of heterogeneous cells
- Produces information used in finite reactor calculations (e.g., DONJON)
- Solves Bateman equations for burnup
- Using customized version to extract fission rates



Fuel Cell

G. Marleau, R. Roy and A. Hébert, *DRAGON: A Collision Probability Transport Code for Cell and Supercell Calculations*, Report IGE-157, Institut de génie nucléaire, École Polytechnique de Montréal, Montréal, Québec (1994)

Why are we excited about DRAGON?

1) It is a multiplatform open-source code.

2) It is *fast*, allowing quick calculations of systematic errors.

It is an order of magnitude faster than MCNP-based code.

But is it accurate enough?

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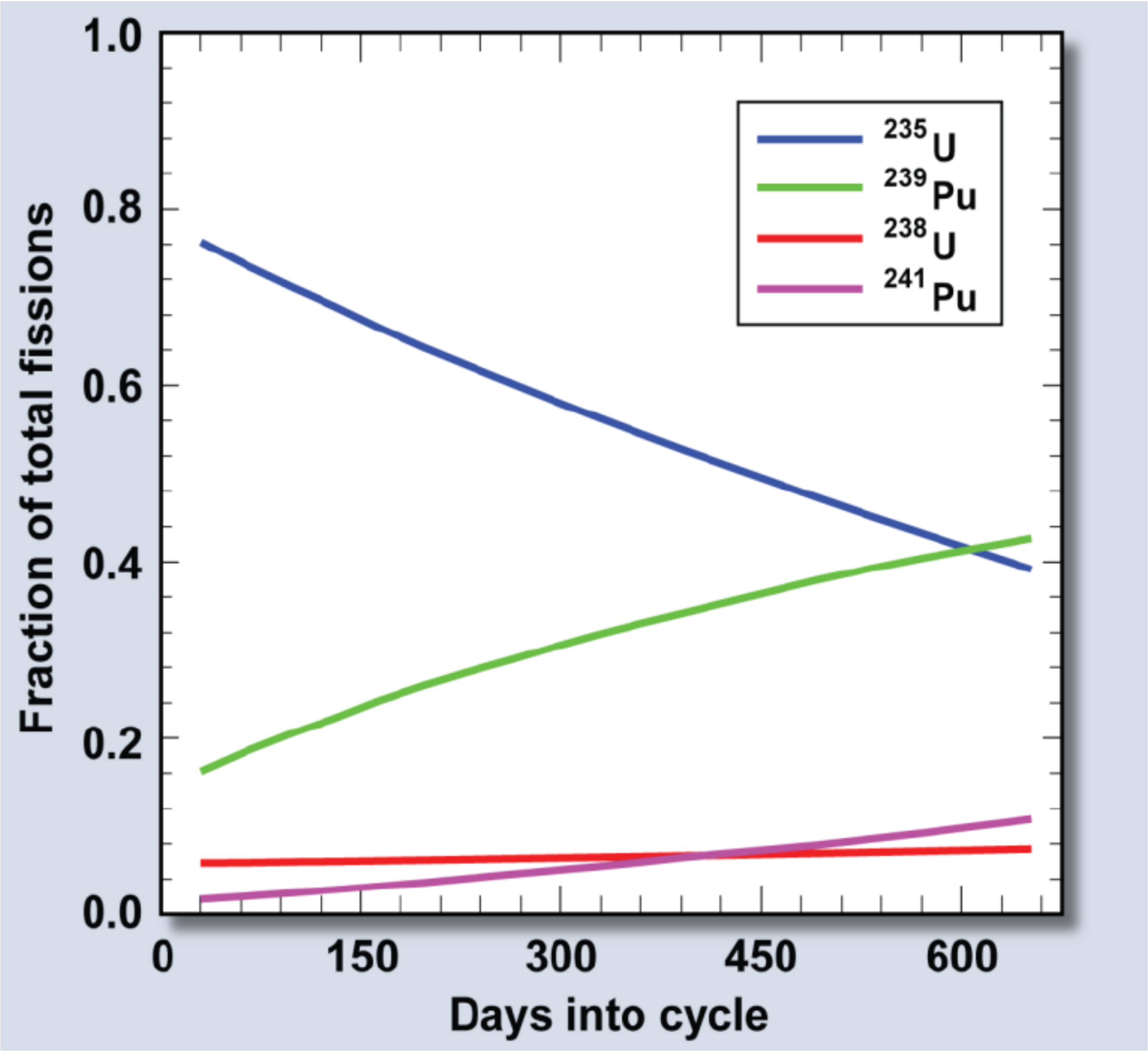
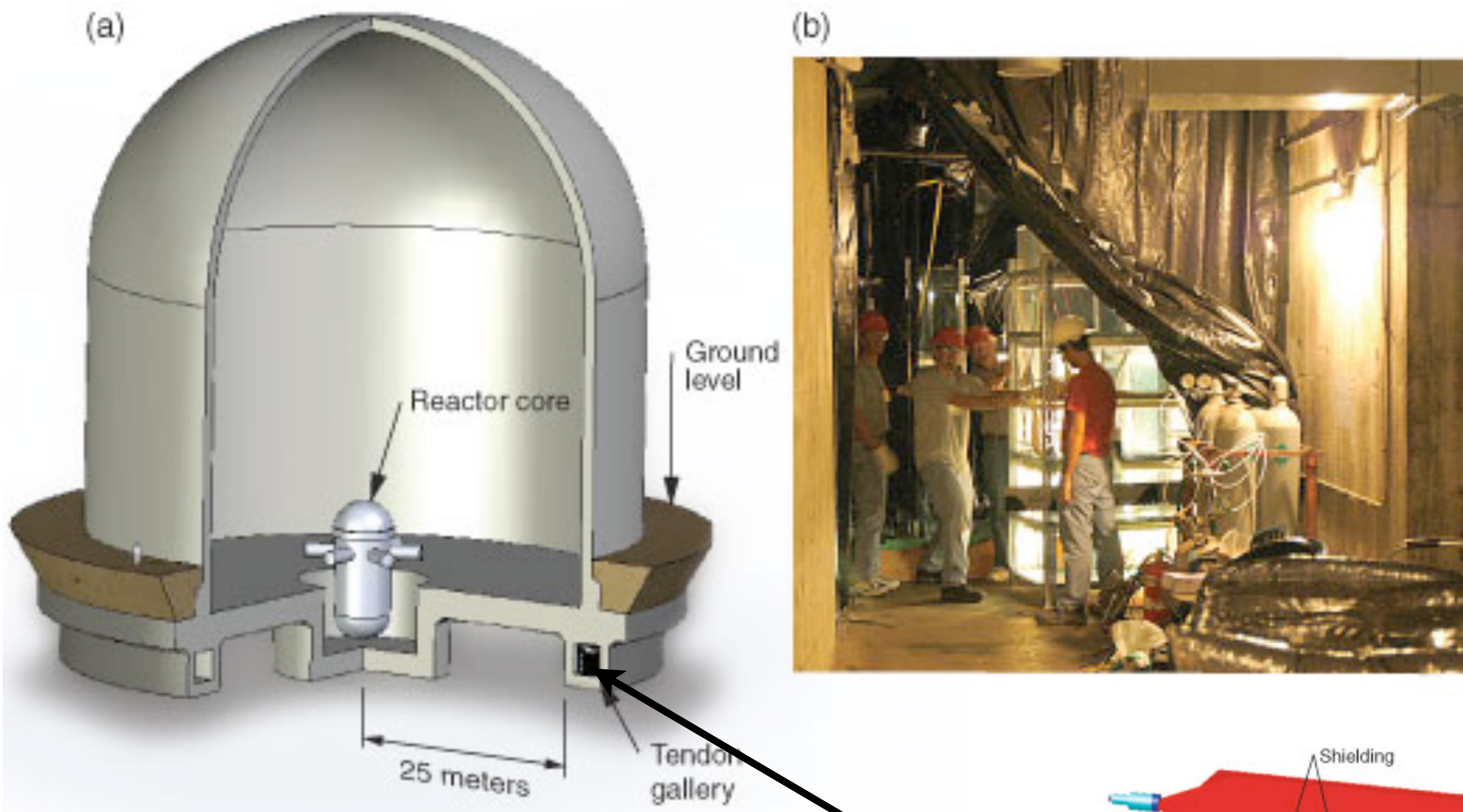
DRAGON test #1: Can we predict the time dependence of the antineutrino flux?



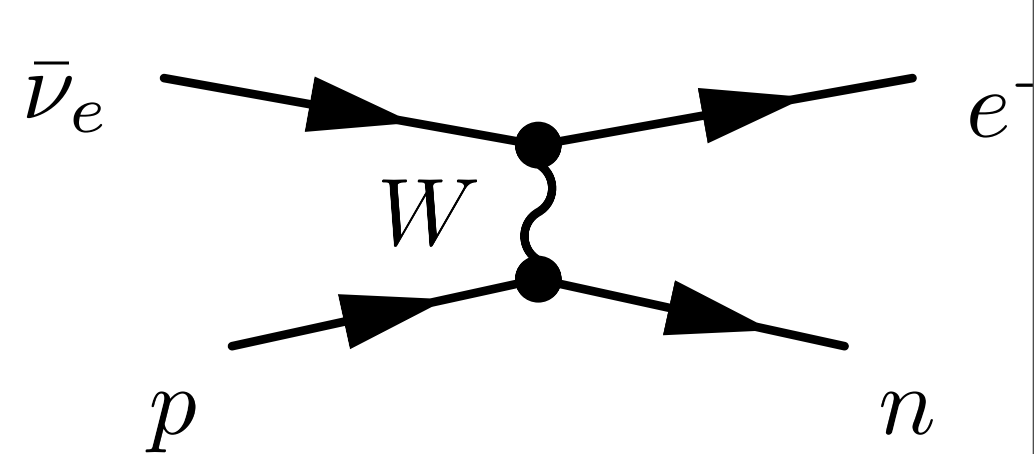
Time dependence is due to changing fissile materials.

SONGS: Detector and Reactor

San Onofre Nuclear Generating Station

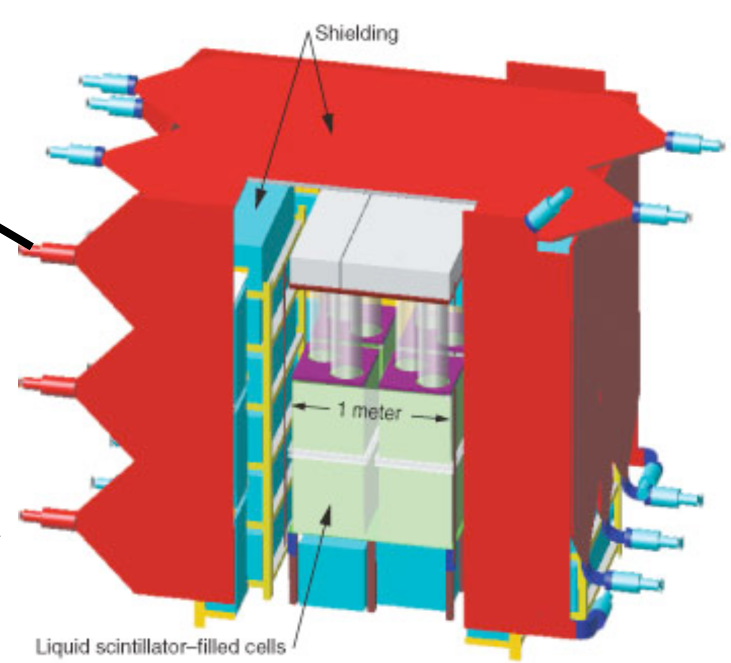


Purpose: joint nonproliferation effort between LLNL and Sandia Laboratory



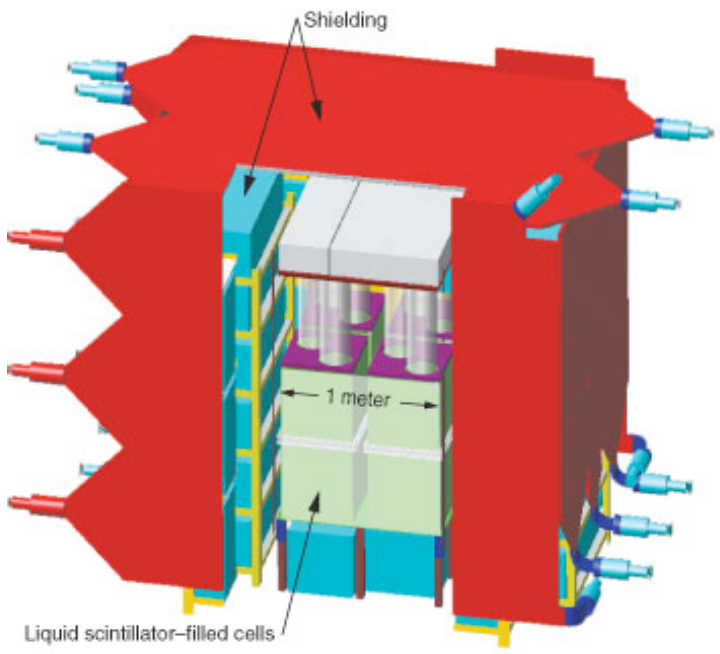
Detection method: Inverse β decay

SONGS reactor: 3.438 GWth output



SONGS detector:
0.64 ton liquid scintillator doped with Gd

Goals of SONGS Detector

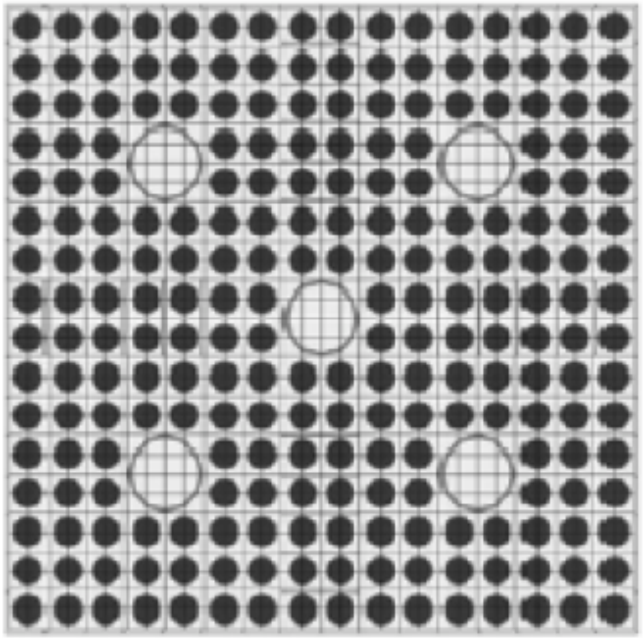


- Detector monitored power and plutonium in the core.
- It counted antineutrino events above threshold (prompt threshold: 2.39 MeV)
- SONGS has an overall uncertainty in the amount of liquid at the 10% level

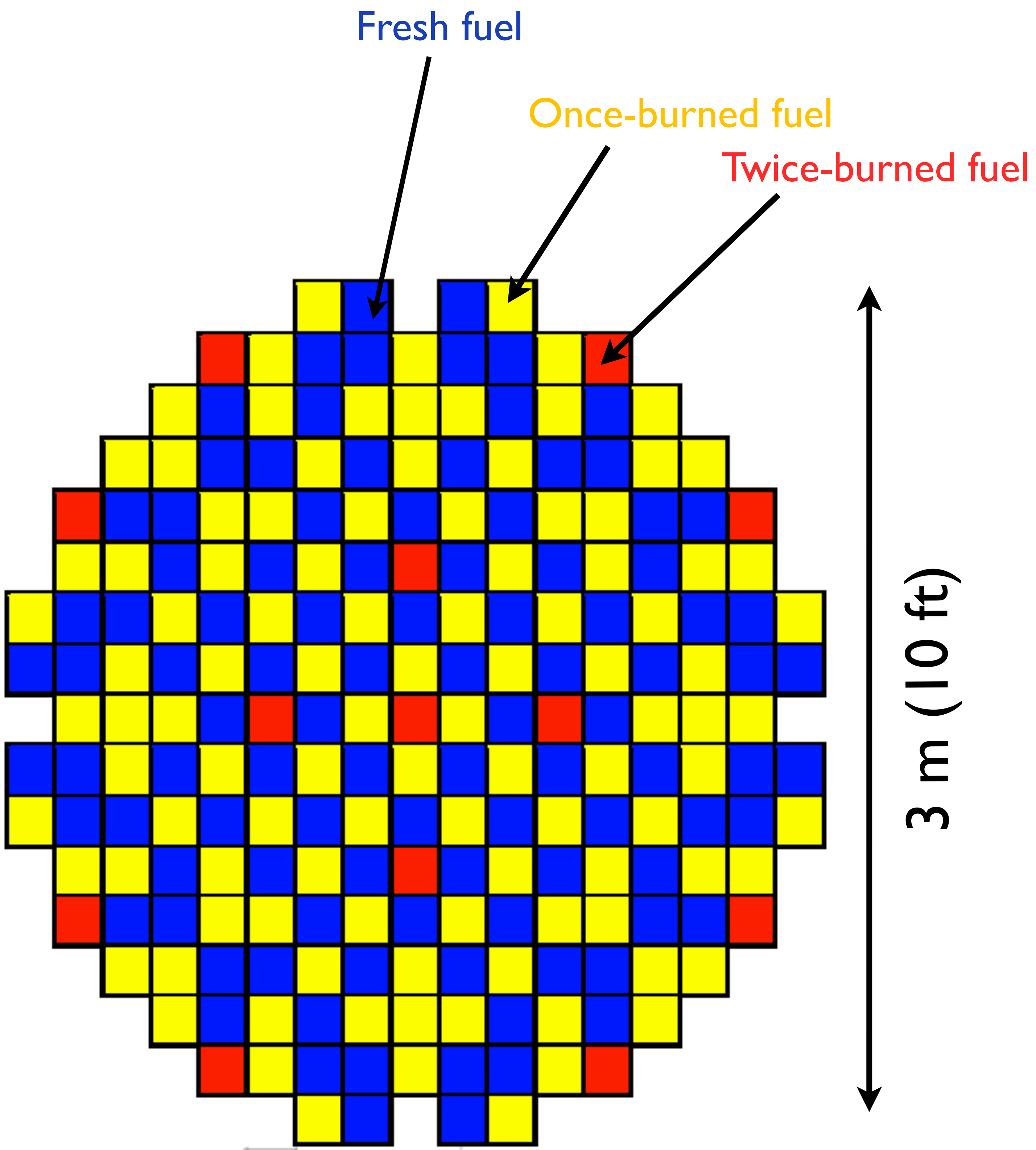
SONGS Reactor Assembly Details

- 16 x 16 PWR
- 236 fuel rods per assembly
- 217 assemblies in the core
- 3.81 m in height

DRAGON simulates assemblies



Westinghouse CE fuel assembly



SONGS Core Map

Calculating the Detected Antineutrino Rate

Sum over primary fissile nuclei

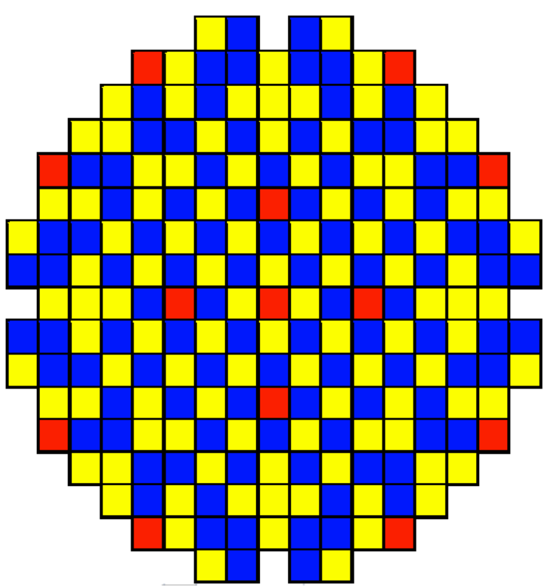
Inverse beta decay cross section

$$\frac{dN_\nu}{dt} = \frac{\epsilon N_p}{4\pi D^2} \sum_i f_i \int_{1.806}^{10} dE_\nu \sigma(E_\nu) S_i(E_\nu)$$

Neutrino spectra

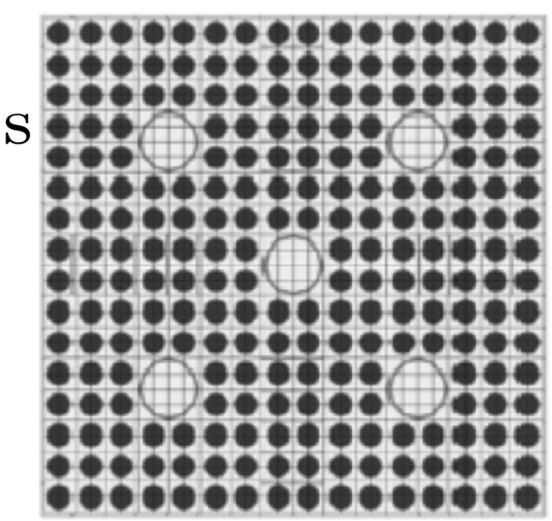
average detection efficiency

fission rate from DRAGON



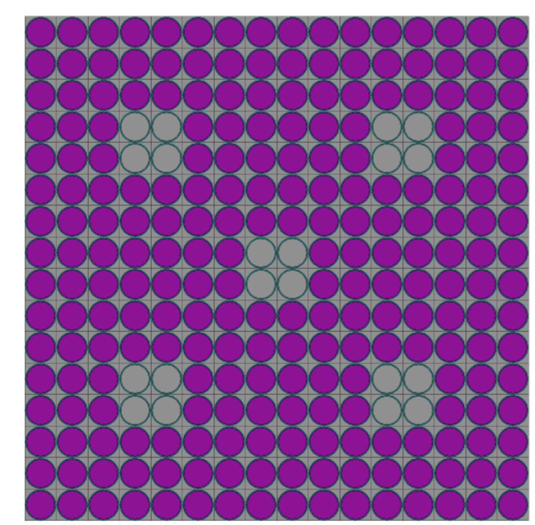
actual SONGS core

$$\approx \sum_i^{\text{assemblies}}$$



Westinghouse 16 x 16 CE assembly

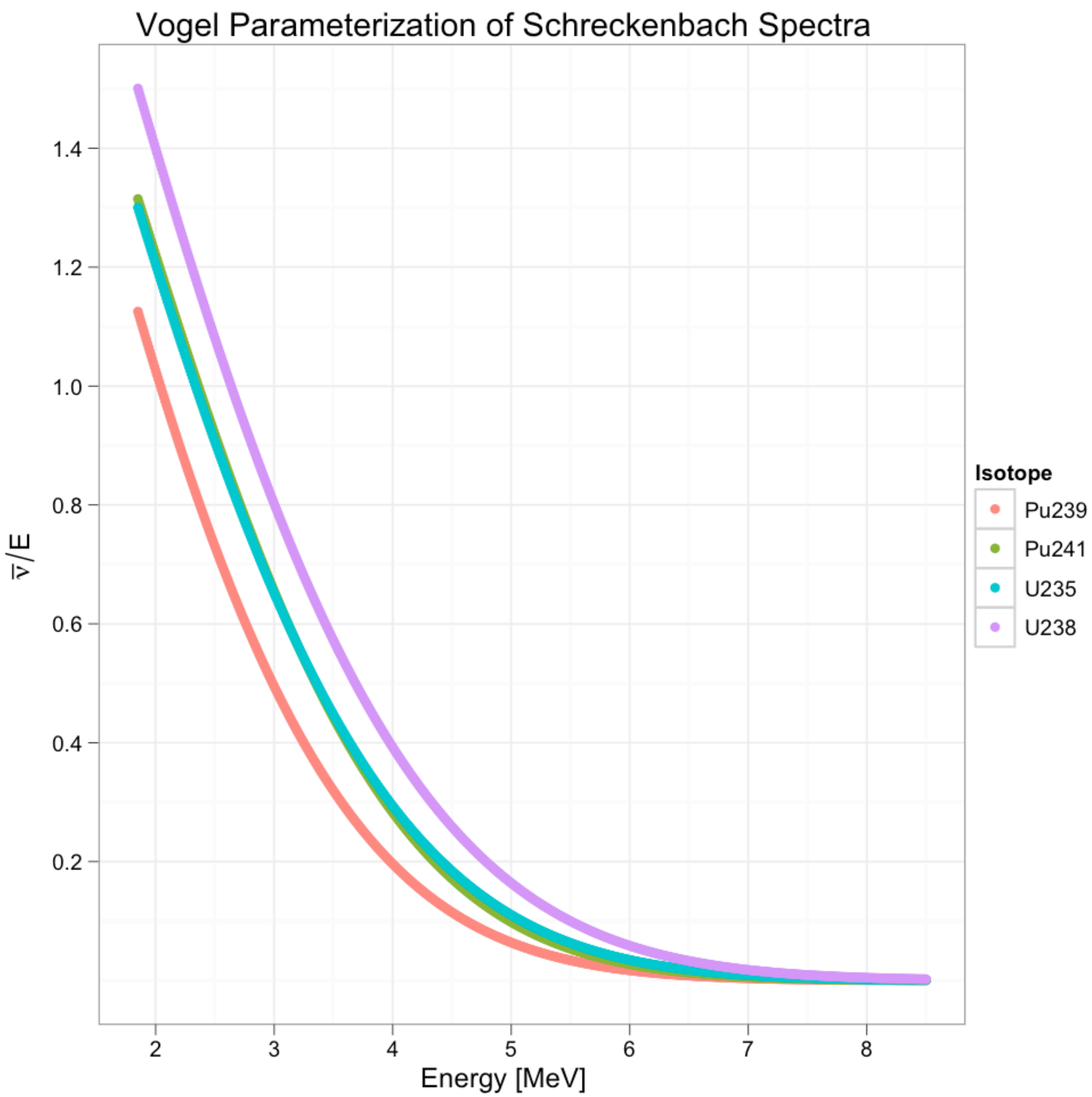
$$\approx \sum_i^{\text{assemblies}}$$



DRAGON assembly

Neutrino Spectra

$$\log \frac{dN_\nu}{dE_\nu}\bigg|_i \equiv S_i(E_\nu) = a_{0i} + a_{1i}E_\nu + a_{2i}E_\nu^2$$



These provide the number of antineutrinos produced per fission, per nuclide.

Petr Vogel provides a parameterization:

P. Vogel and J. Engel, Phys. Rev. D 39, 3378 (1989)

As of January, there is a new spectrum prediction; how does that affect this work?

1) The normalization is shifted by 3%.

2) The time dependence that we are studying here remains unaffected.

3) Energy dependence of the spectra agree to within less than 2%.

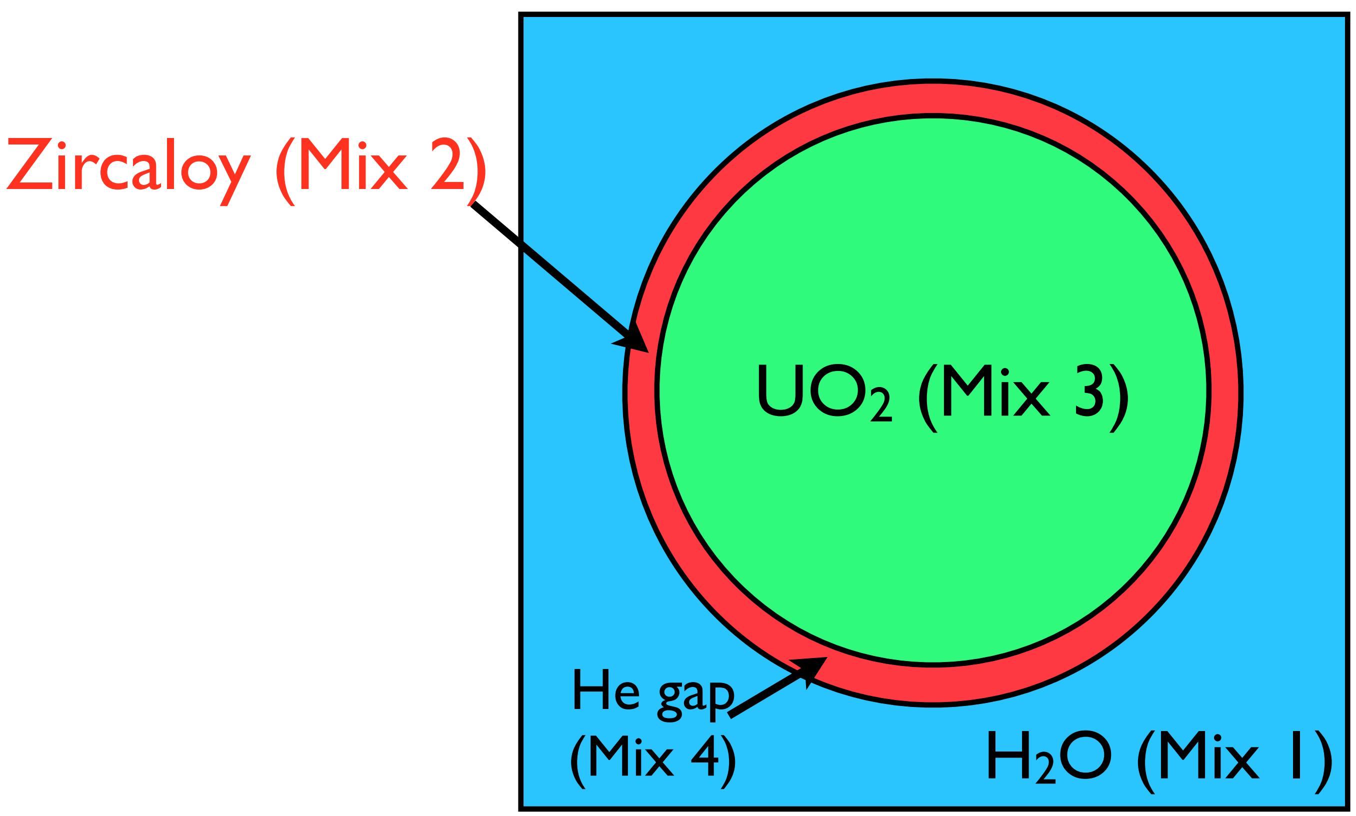
References: arXiv:1101.2663, 1101.2755v3

Inputs to DRAGON: Mixtures

Sample from DRAGON input file

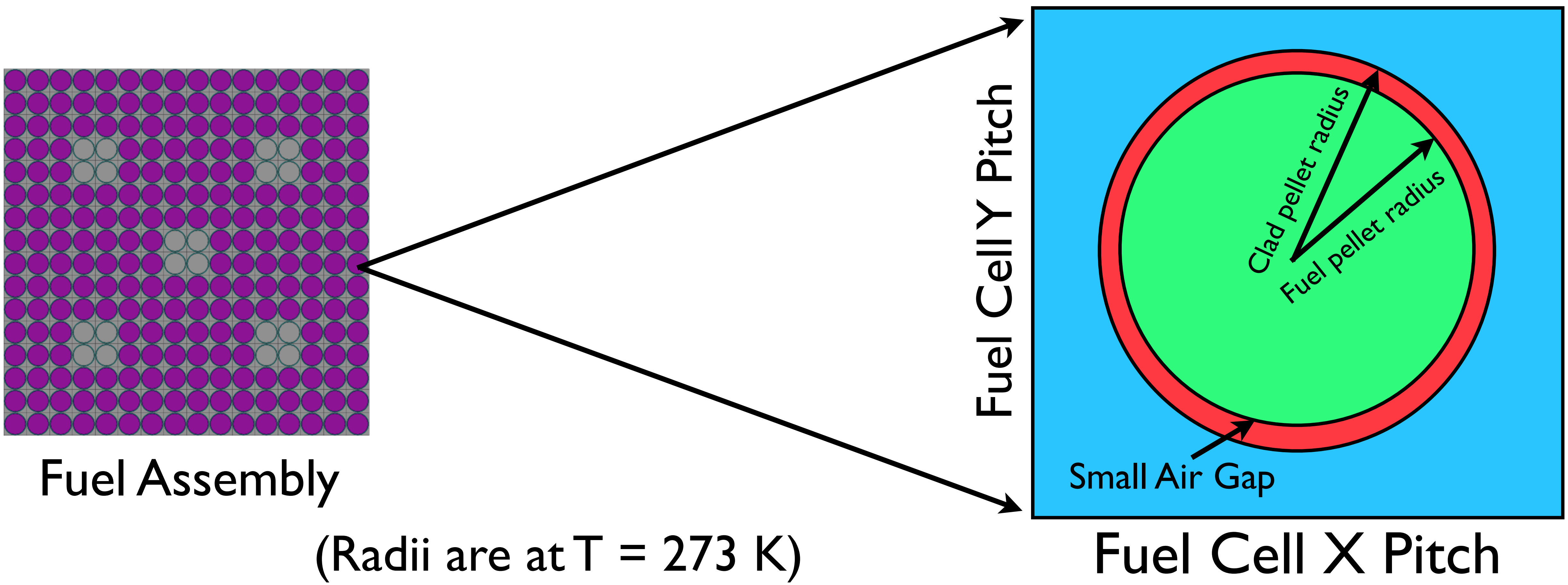
```
MIX 1 578.9 0.713
   H1H2O    = '3001'   11.09
   O16H2O   = '6016'   88.9
   BNat     = '1011'   600E-4
MIX 2 578.9 6.56
  CrNat     = '52' 0.100
  FeNat     = '2056' 0.210
  ZrNat     = '91' 98.23
  SnNat     = '118' 1.45
  HfNat     = '178' 0.010
MIX 3 773.0000 10.2958438186655
  O16      = '6016'  0.1202
  U235     = '2235'   1.23139210364806 1
  U238     = '8238'   86.7498526944542 1
  Pu238    = '948'    0.0140 1
  Pu239     = '6239'   0.5650 1
  Pu240     = '1240'   0.2030 1
  Pu241     = '1241'   0.1270 1
  Pu242     = '242'   0.0400 1
  U234     = '234'   0.0200 1
  U236     = '236'   0.4800 1
  Np237     = '937'  0.046140 1
  Np239     = '1939'   0.0 1
  Am241     = '951'  0.003670 1
  Am242m     = '952'   0.0 1
  Am243     = '953'   0.0 1
  Cm242     = '962'   0.001185 1
  Cm243     = '963'   0.0 1
  Cm244     = '964'   0.001834 1
MIX 4 773.0000
  He4       = '4'    0.00034043
;
```

(data courtesy Southern California Electric)



The fuel composition and temperature vary by assembly.

Inputs Into DRAGON: Geometry



(Radii are at T = 273 K)

X Pitch	Y Pitch	Pellet Radius	Helium Gap Radius	Cladding Radius
1.265 cm	1.265 cm	0.4134 cm	0.422 cm	0.485 cm

SONGS Parameters

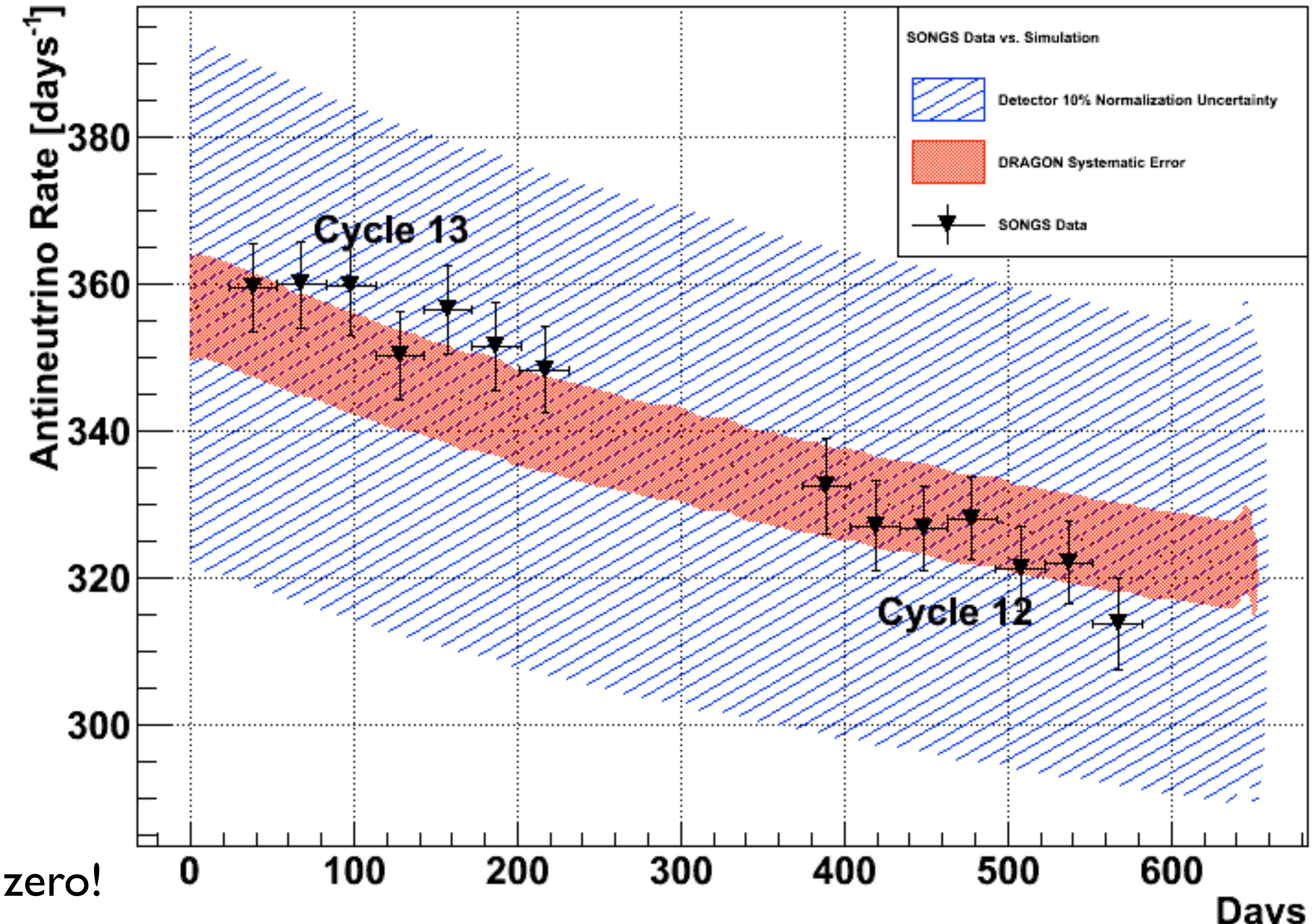
Because of this, we won't be able
normalize our data, but we can test
time dependence

detection efficiency	distance to reactor	Number of target protons
10% +/- 1%	24.5 +/- 1.0 m	4.35E+28

Nuclear Instruments and Methods in Physics Research A 572 (2007) 985-998

$$\frac{dN_\nu}{dt} = \frac{\epsilon N_p}{4\pi D^2} \sum_i f_i \int_{1.806}^{10} dE_\nu \sigma(E_\nu) S_i(E_\nu)$$

DRAGON Prediction for Cycle 12



Take away: time dependence agrees well!

Suppressed zero!

-Assume 2% uncertainty on thermal power (red band); only Cycle 12 shown here for clarity

-Assume 10% uncertainty on efficiency (blue band)

Talk Outline

- Example Motivation: Oscillation Experiments
- Overview of Double Chooz Detector
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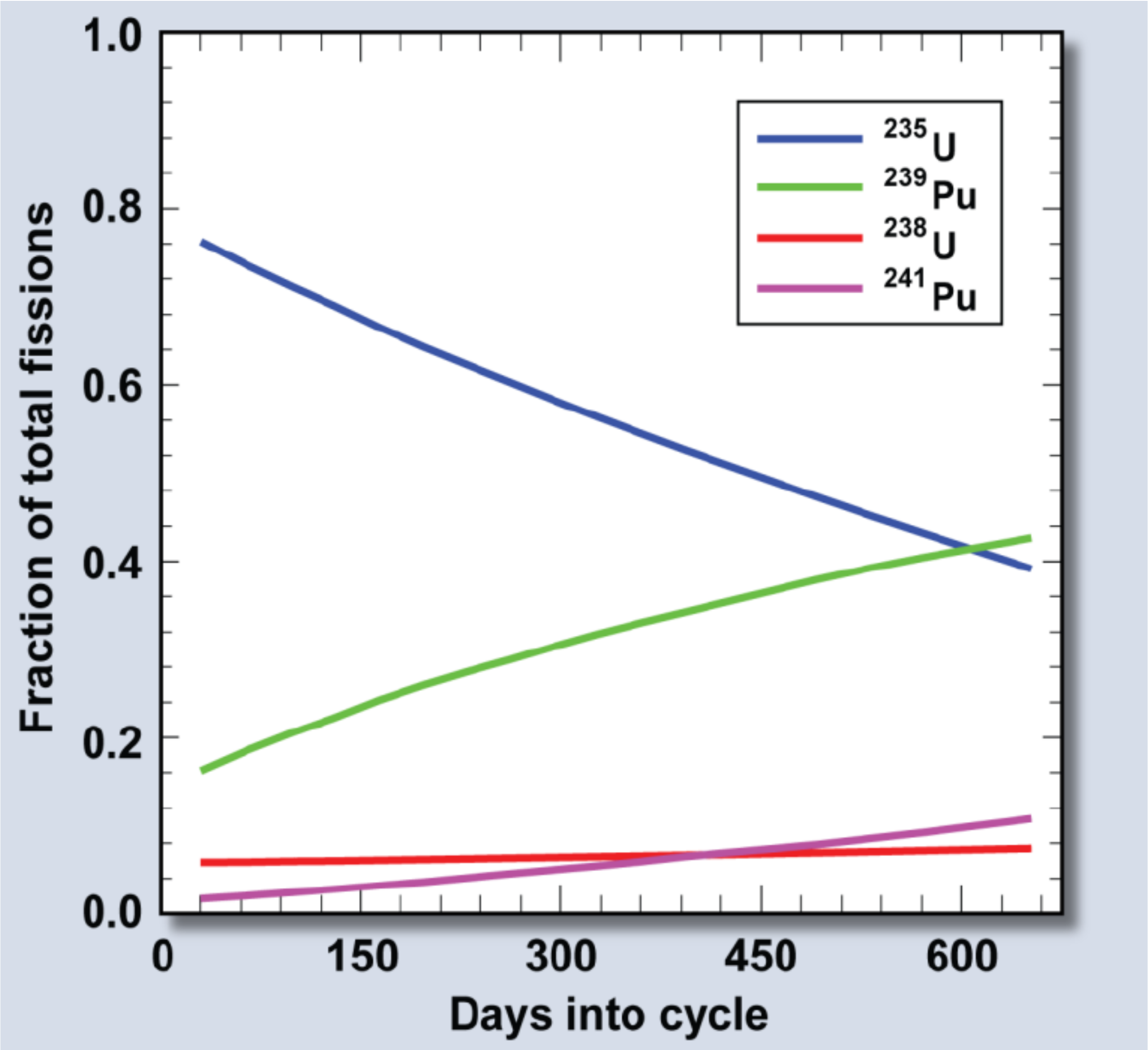
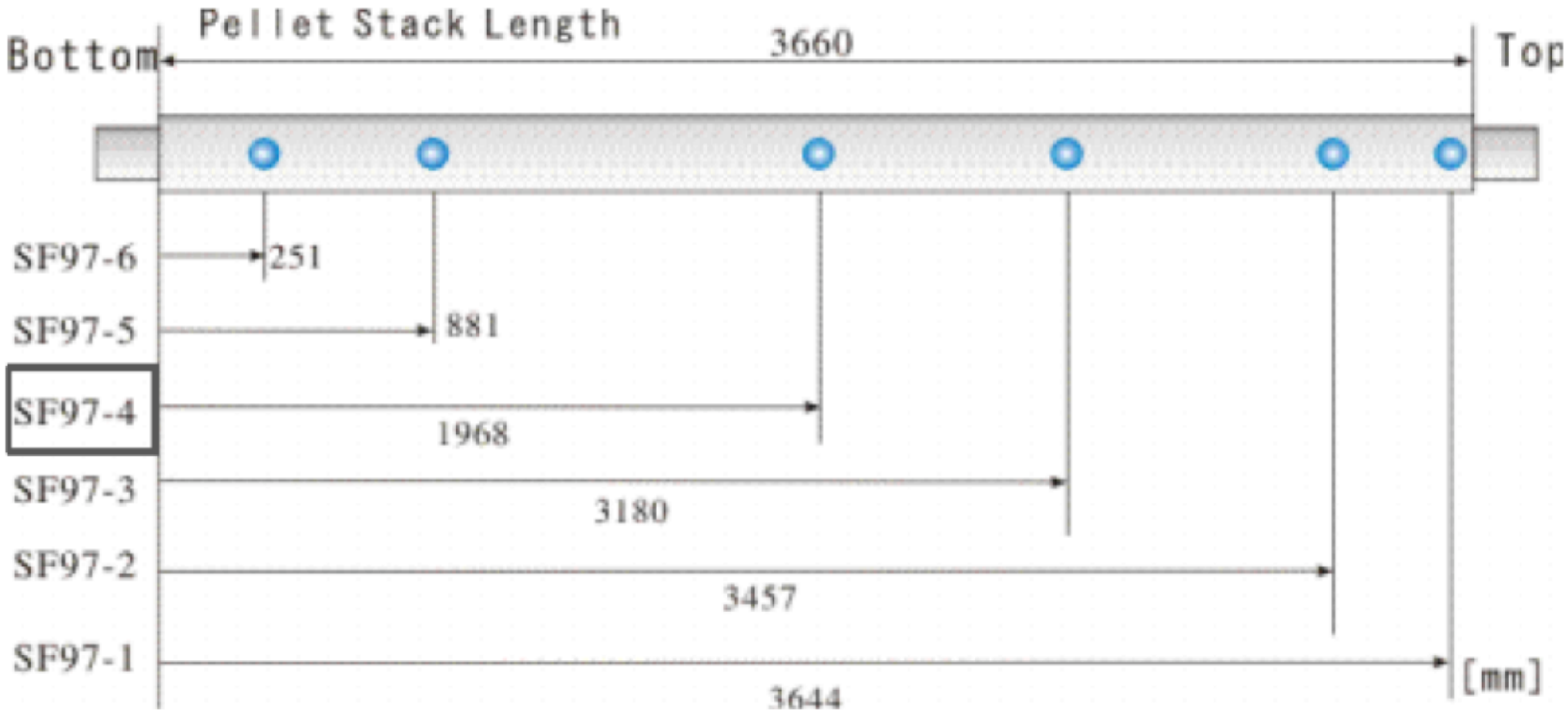
DRAGON Test #2: Are we sure that we get the fissile inventory right?



What Is the Takahama Benchmark?

- The Takahama-3 reactor is a 17 x 17 PWR in Japan.
- They removed some fuel rods for a destructive assay from 2 of the assemblies.
- The results are publicly available!
- We (and many others) can compare our simulations to what they found!
- This is a very valuable method that allows us to assign systematic errors in DRAGON's fission rate and mass inventory predictions.

Destructive Assay of Fuel Rods



After the reactor was shut down, the fuel rods in the benchmark underwent a chemical analysis.

From each rod, the fuel amounts along the axis were extracted at several points. Shown here is rod SF97.

Takahama-3 Reactor Assembly Details

17 x 17 PWR

264 rods per assembly

217 assemblies in the core

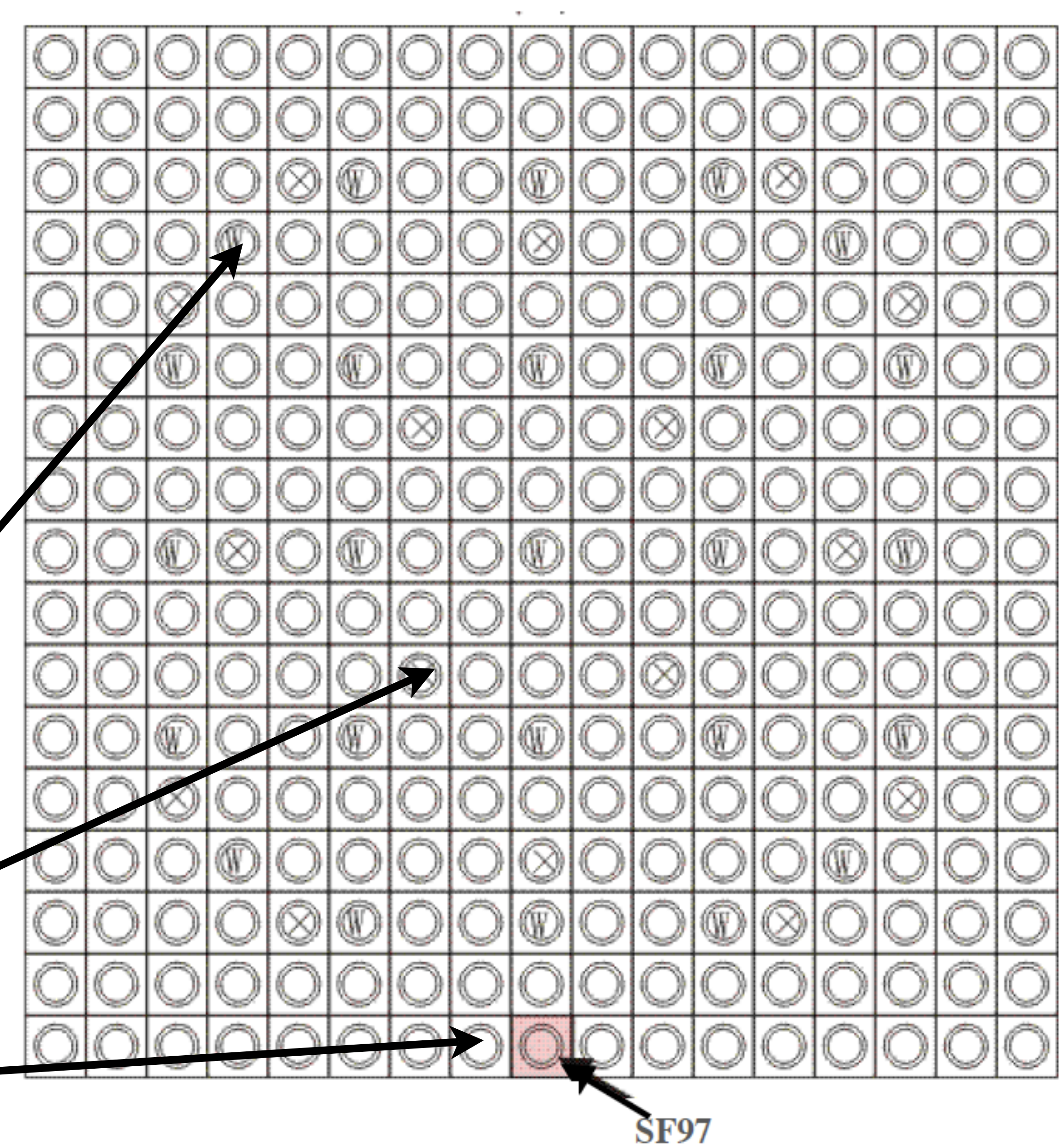
3.66 m in height

2.652 GWth

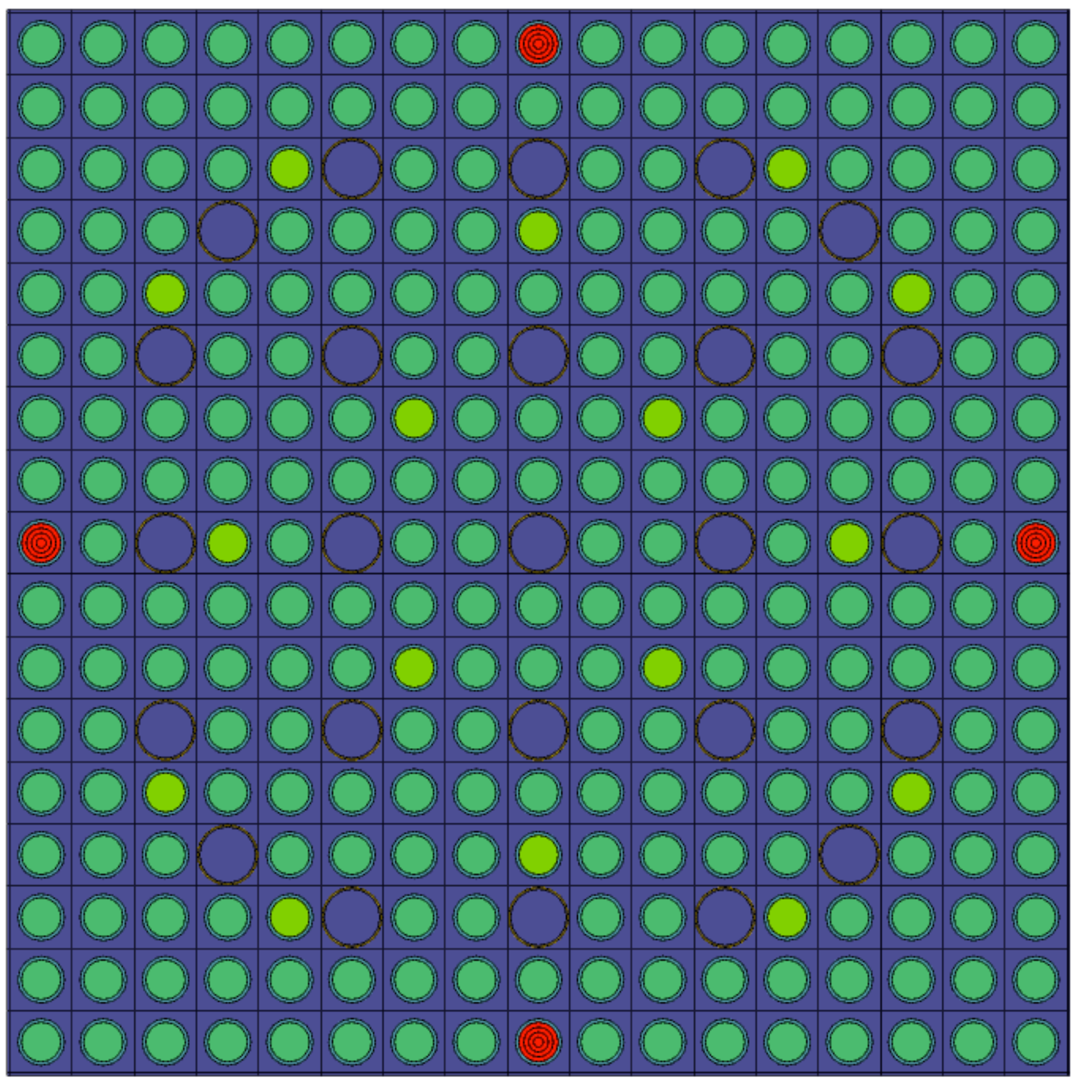
guide tube filled with borated water

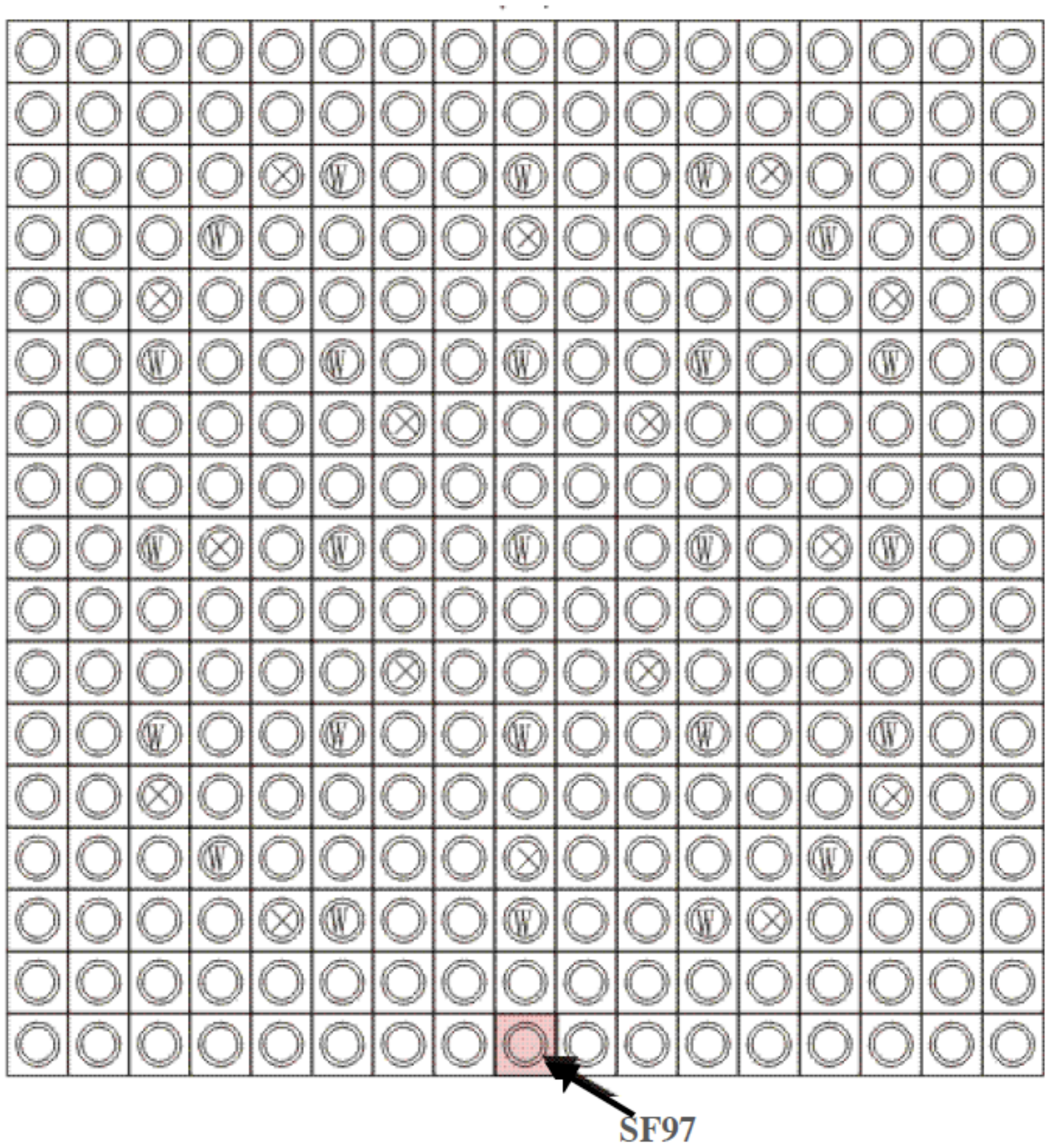
2.63% enriched Gd-U burnable absorber rod

4.11% enriched fuel rod



Takahama-3 Assembly NT3G24





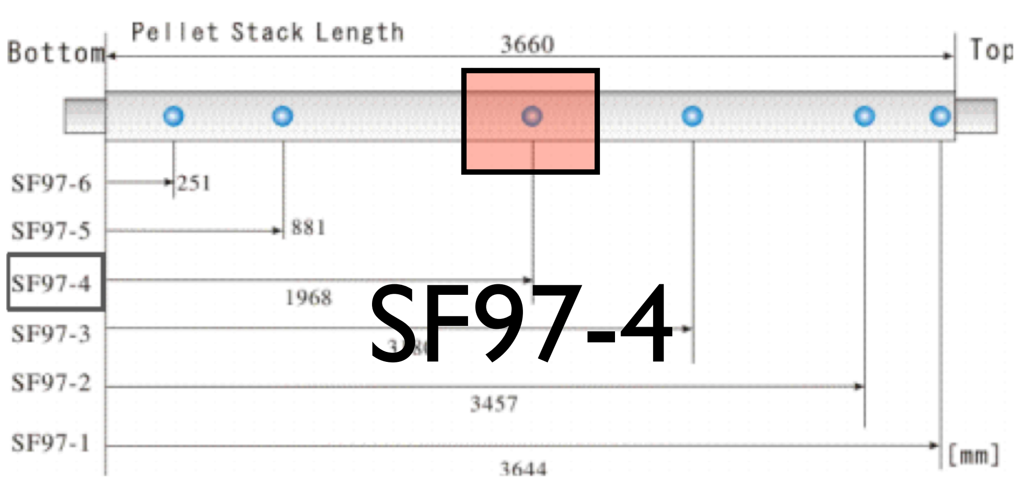
Irradiation Times

Start	Stop	Days	Status	Cycle
1990/01/26	1991/02/15	385	Burnup	5
1991/02/15	1991/05/14	88	Cool	
1991/05/14	1992/06/19	402	Burnup	6
1992/06/19	1992/08/20	62	Cool	
1992/08/20	1993/09/30	406	Burnup	7

The reactor was evolved for 1343 days.

Takahama-3 Benchmark Results: Calculated / Measured

Isotope	DRAGON	SCALE	HELIOS
U235	0.98	0.97	1.02
U238	1.00	1.00	1.00
Pu239	0.99	0.99	1.03
Pu241	0.97	0.96	1.02

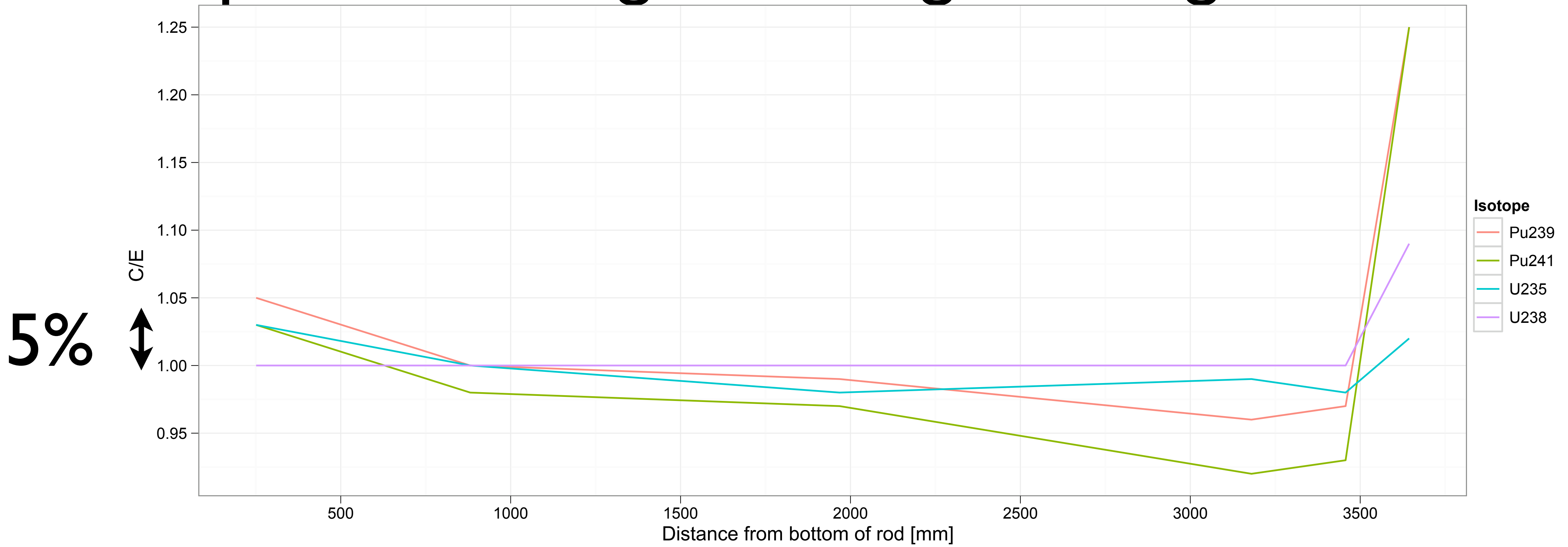


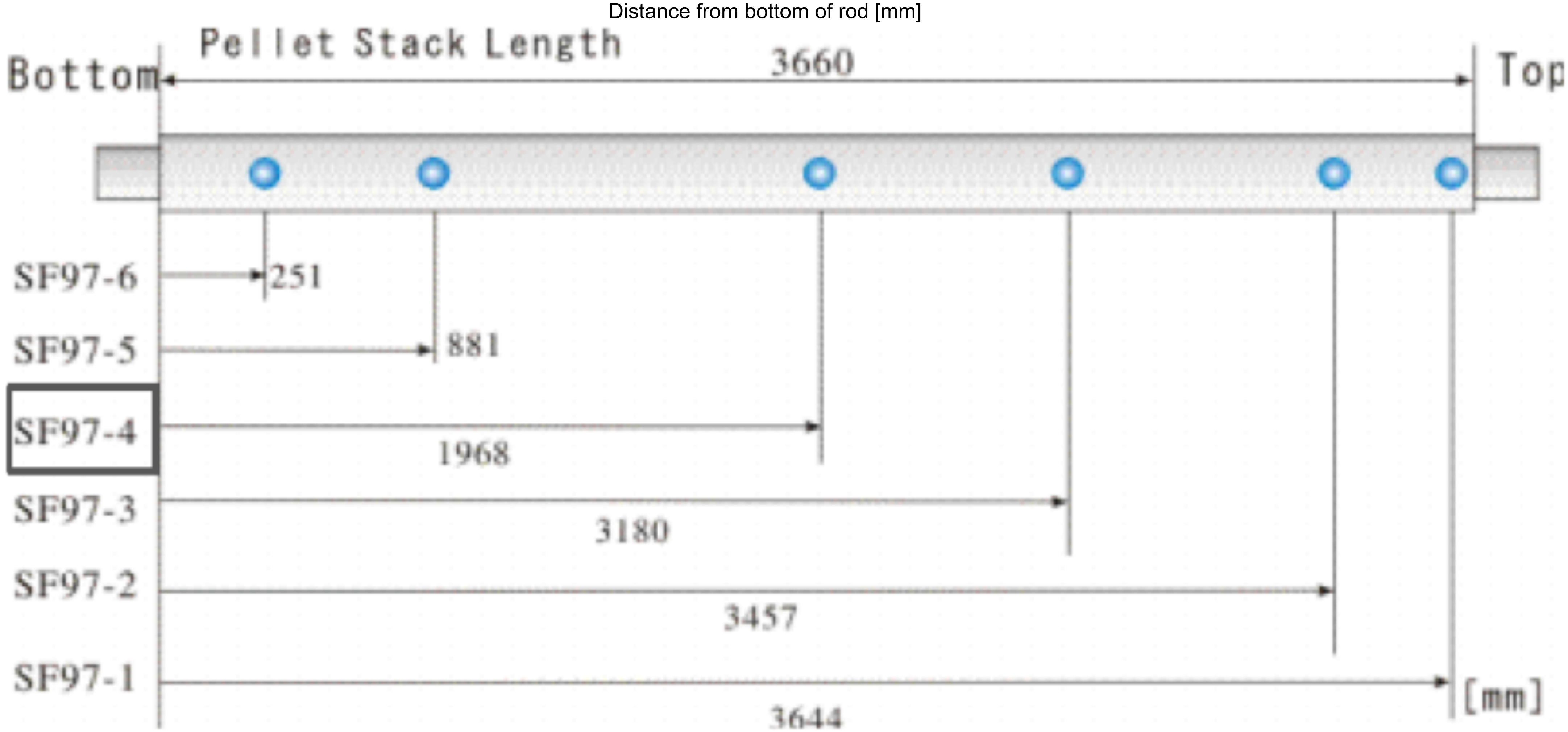
This comparison is for fuel at the center of the rod.

Take away: open-source code DRAGON is as good as proprietary codes used by industry!

Isotope	DRAGON	SCALE	HELIOS
U235	0.98	0.97	1.02
U238	1.00	1.00	1.00
Pu239	0.99	0.99	1.03
Pu241	0.97	0.96	1.02

Our prediction is good along the length of the rod.





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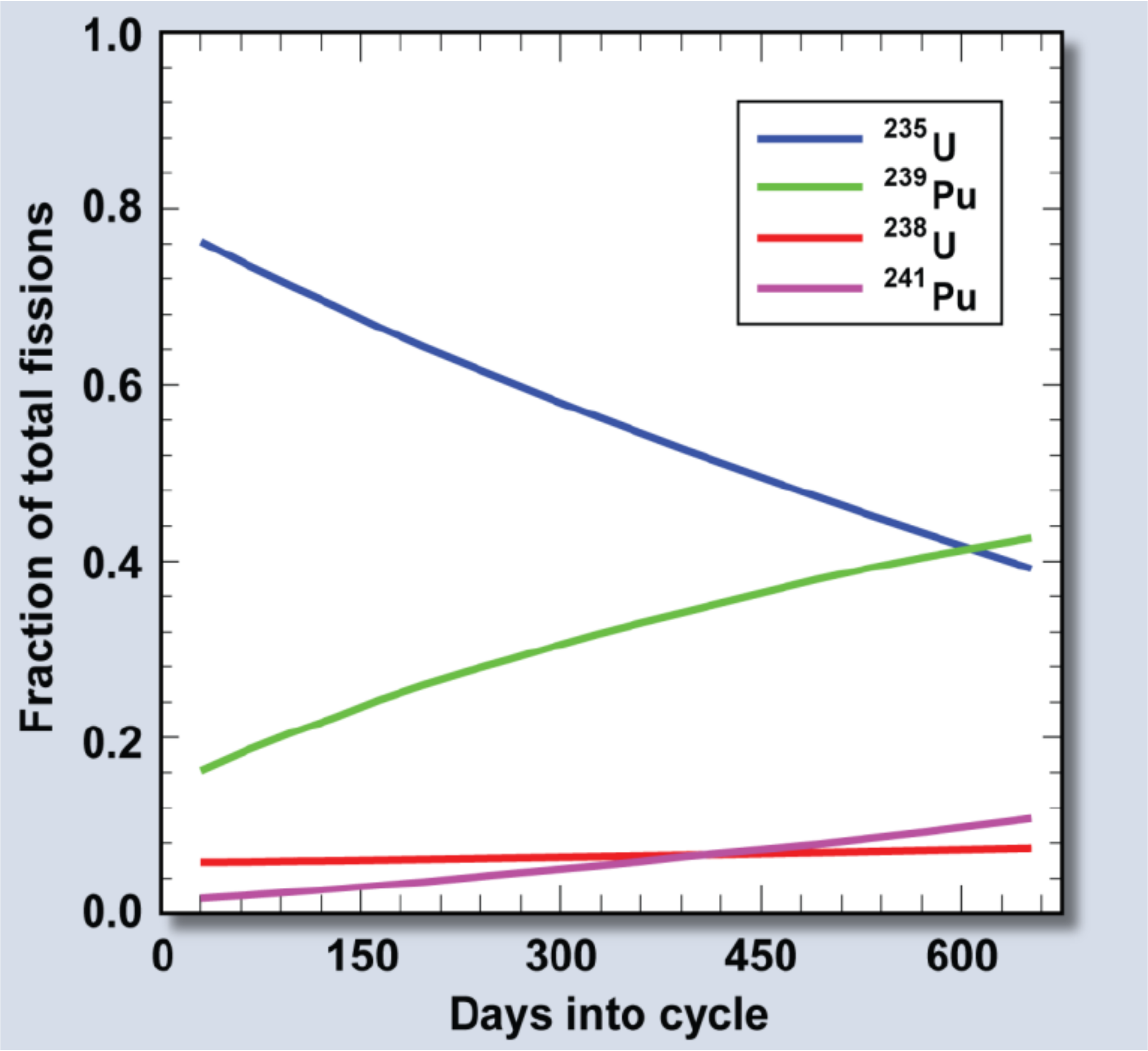
Application for DRAGON: Can we test the fissile inventory of a reactor in real time?



Central Issue For Nuclear Nonproliferation

How does one balance a nation's need for electrical power and research with nuclear reactors with the possibility of weapons production?

N. Korea Reports Advances in Enriching Uranium

By DAVID E. SANGER
Published: September 3, 2009

WASHINGTON — North Korea declared Friday that it was in the "concluding stage" of tests to enrich uranium. Its statement would appear to end a decade-long debate within American intelligence agencies about whether the country was working on a second pathway to building nuclear weapons.

A Defiant Iran Vows to Build Nuclear Plants

By DAVID E. SANGER and WILLIAM J. BROAD
Published: November 29, 2009

WASHINGTON — Iran angrily refused Sunday to comply with a demand by the United Nations nuclear agency to cease work on a once-secret nuclear fuel enrichment plant, and escalated the confrontation by declaring it would construct 10 more such plants.

Most monitoring techniques require cooperation

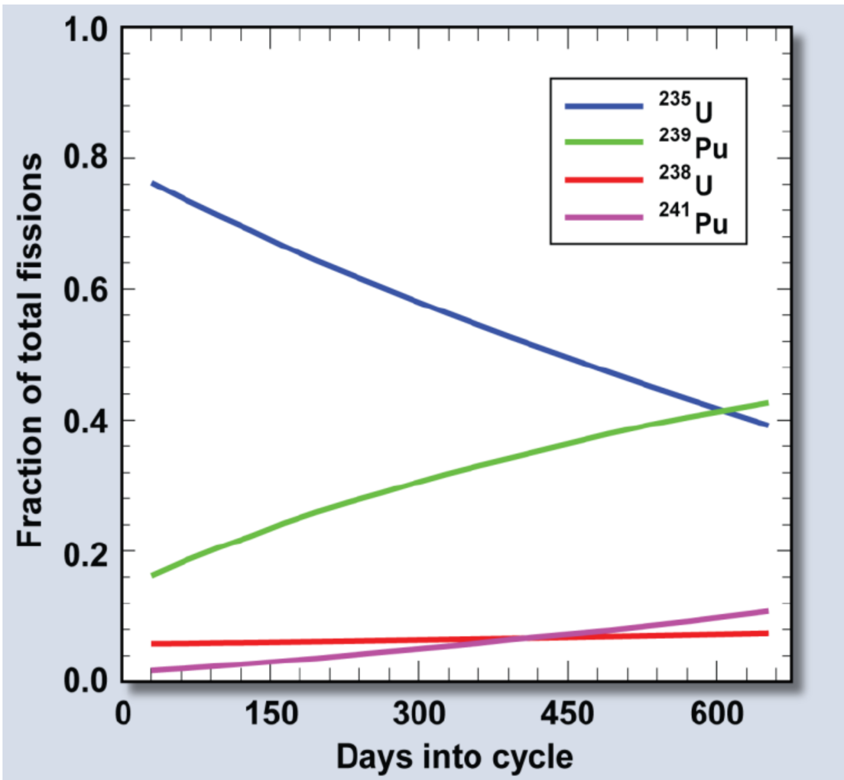
- Cameras
- Thermal monitoring: monitors have to be attached to pipes. Electrical monitoring is not sufficient.
- Detection of materials involved in reprocessing
- Analysis of plutonium samples

But techniques which are non-intrusive are better

e.g. Detection of emission of xenon and krypton-85

Antineutrino detection allows real-time and non-intrusive assay for the entire core.

The Need For Nonintrusive Detection



PWRs consume uranium and produce plutonium.

PWRs operate at constant power.

What happens if someone "diverts" spent plutonium after a fuel cycle?

Power = P

X kg of uranium

Y kg of plutonium

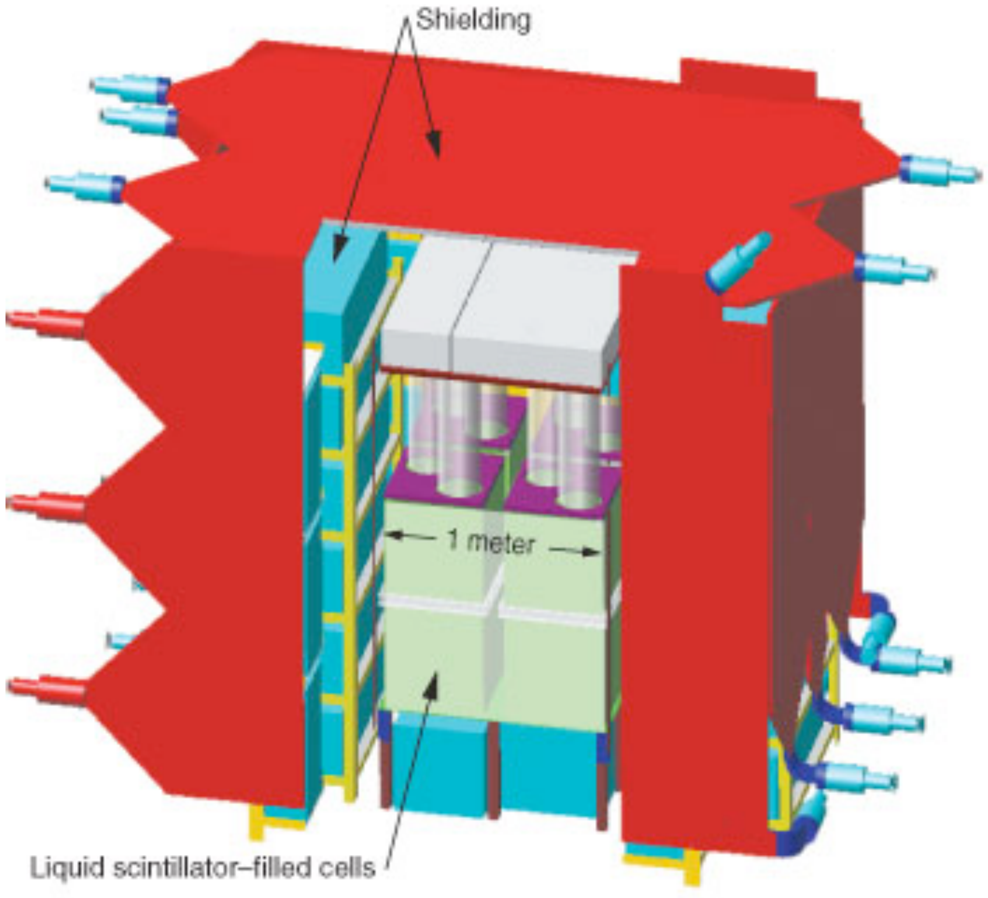
Power = P

X + 200 kg of uranium

Y - 50 kg of plutonium

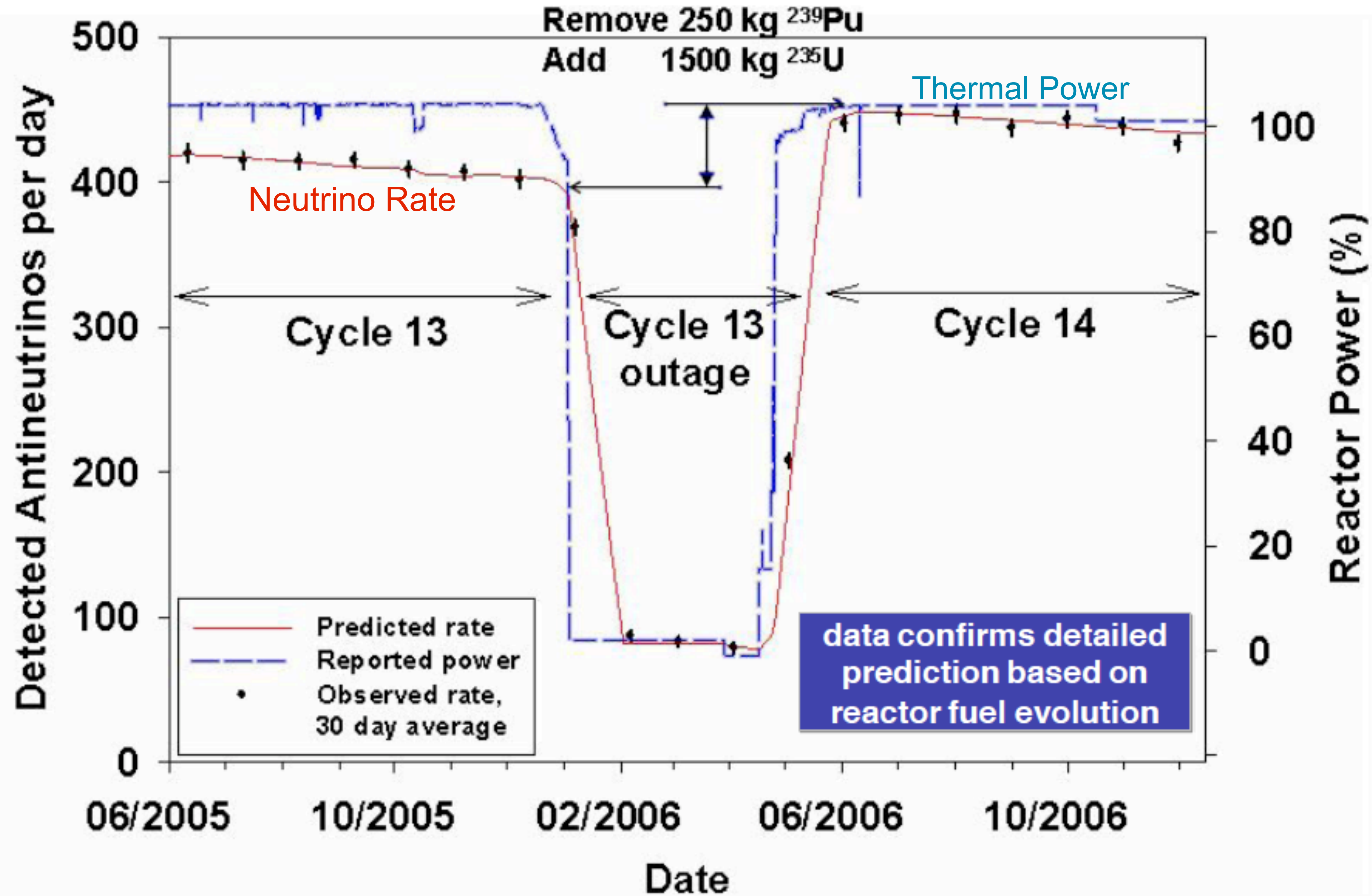
How To Use Antineutrinos For Nonintrusive Monitoring

- Use a small (cubic-meter or smaller) detector near the reactor, or...
- ...be "outside the fence" (but large).
- Recognize that different fissile isotopes contribute differently to the total rate and flux.
- Bernstein et. al. have shown that this is feasible with SONGS!



See: arXiv:1009.2123

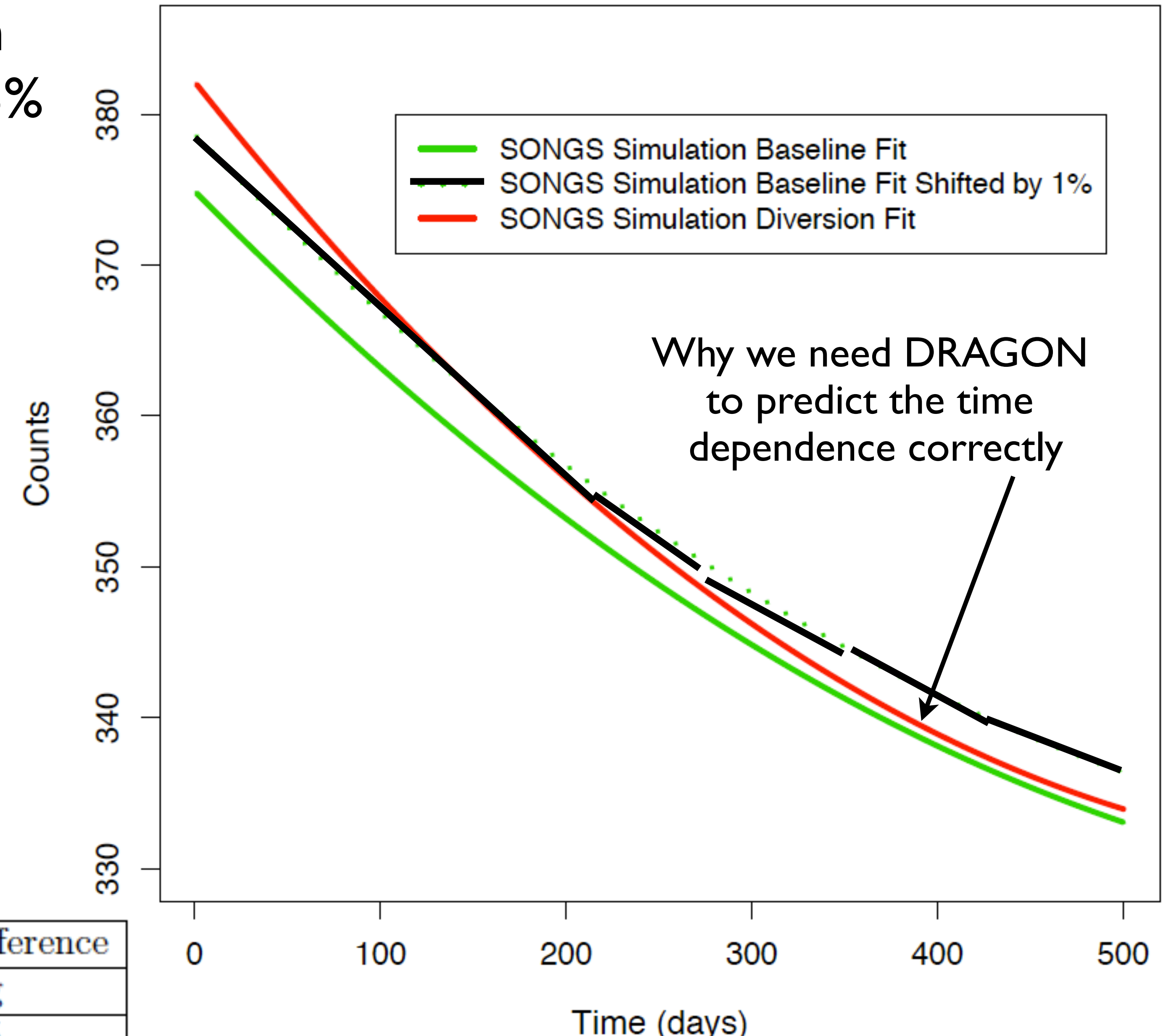
Test for Diversion



Statistical procedure developed at LLNL can detect 72 kg Pu diversion in 90 days with 95% confidence.

Procedure depends on counting statistics and overall systematic shift in power.

Can we improve upon the ORIGEN reactor simulations?



	Baseline mass (kg)	Diversion scenario mass (kg)	Mass difference kg
^{235}U	2834	2849	15
^{238}U	82912	83351	439
^{239}Pu	226	152	-74
^{241}Pu	21	12	-9

A plutonium weapon can contain as little as 5 - 10 kg of refined plutonium!

Summary

- Reactor simulations are important for particle physics.
  We recommend DRAGON as your simulation code!
- The SONGS and Takahama benchmarks show that DRAGON, which is open source and fast, can predict fissile inventory as well as proprietary codes.
- The application of DRAGON to nonproliferation studies looks promising.

Double Chooz Systematics

		Chooz	Double Chooz
Reactor	ν flux and spectrum	1.9%	<0.1%
	Reactor Power	0.7-2%	<0.1%
Detector	Solid Angle	0.3%	<0.1%
	Target Mass	0.3%	0.2%
	Density	0.3%	<0.1%
	H/C and Gd ratio	1.2%	<0.2%
	Spatial Effects	1.0%	<0.1%
	Live time	-	<0.2%
Analysis	From 3-7 cuts.	1.5%	0.2-0.3%
	Total	2.7%	<0.6%

Recent re-analysis of reactor antineutrino spectra conversion procedure

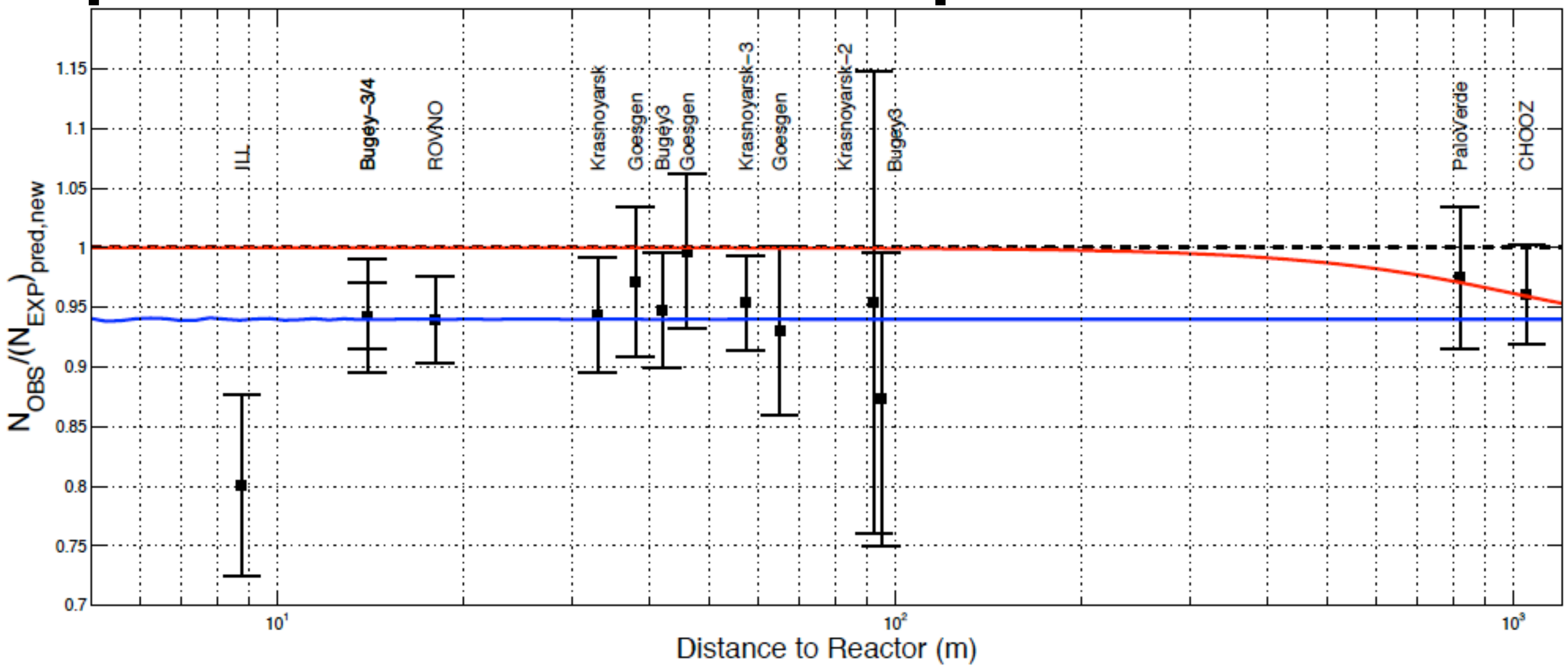


FIG. 4. Illustration of the short baseline reactor antineutrino anomaly. The experimental results are compared to the prediction without oscillation, taking into account the new antineutrino spectra, the corrections of the neutron mean lifetime, and the off-equilibrium effects. Published experimental errors and antineutrino spectra errors are added in quadrature. The mean averaged ratio including possible correlations is 0.937±0.027. The red line shows a 3 active neutrino mixing solution fitting the data, with $\sin^2(2\theta_{13}) = 0.06$. The blue line displays a solution including a new neutrino mass state, such as $|\Delta m^2_{new,R}| \gg 1$ eV^2 (for illustration) and $\sin^2(2\theta_{new,R})$=0.16.

arXiv:1101.2663, 1101.2755v3